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=> dis his

     (FILE 'HOME' ENTERED AT 14:16:53 ON 08 AUG 2006)

     FILE 'REGISTRY' ENTERED AT 14:17:15 ON 08 AUG 2006
L1                STR
L2              5 S L1
L3            126 S L1 FUL
L4                STR L1
L5             65 SEARCH L4  SUB=L3 FUL
L6                STR L4
L7             65 SEARCH L6  SUB=L5 FUL

=> d l7 que stat;fil medl,biosis,embase,caplus;s l7
L1                STR
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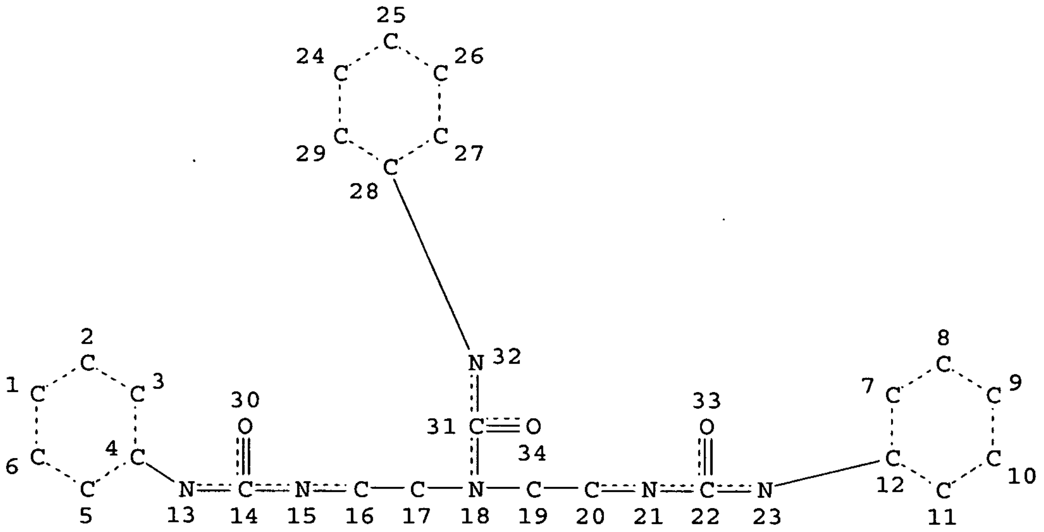

25
24
26
29
27
28
C
N 32
O
31
34
30
33
1
2
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9
10
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17
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19
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21
22
23
N

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  34

STEREO ATTRIBUTES: NONE
L3            126 SEA FILE=REGISTRY SSS FUL L1
L4                STR
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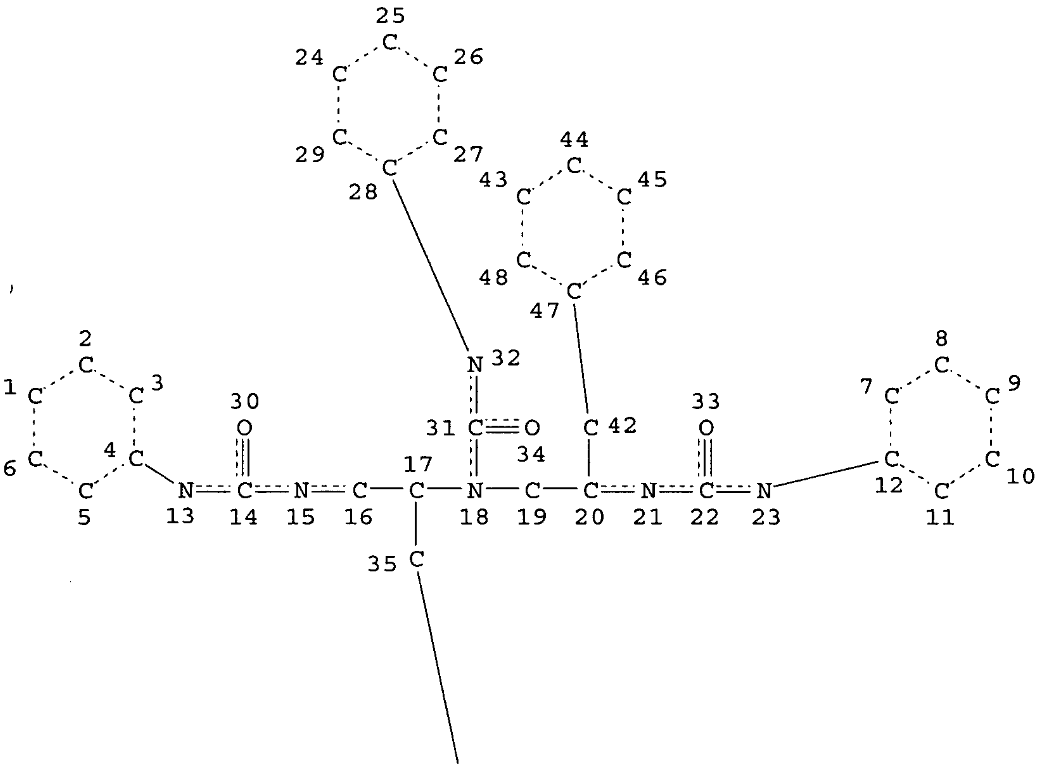
Page 2



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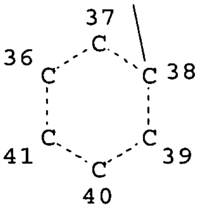
10
11
12
N 32
31 C=O
34
30
O
33
O
C 42
N 13
C 14
N 15
C 16
C 17
N 18
C 19
C 20
N 21
C 22
N 23
35 C

Page 1-A



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Page 2-A

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
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L6               STR
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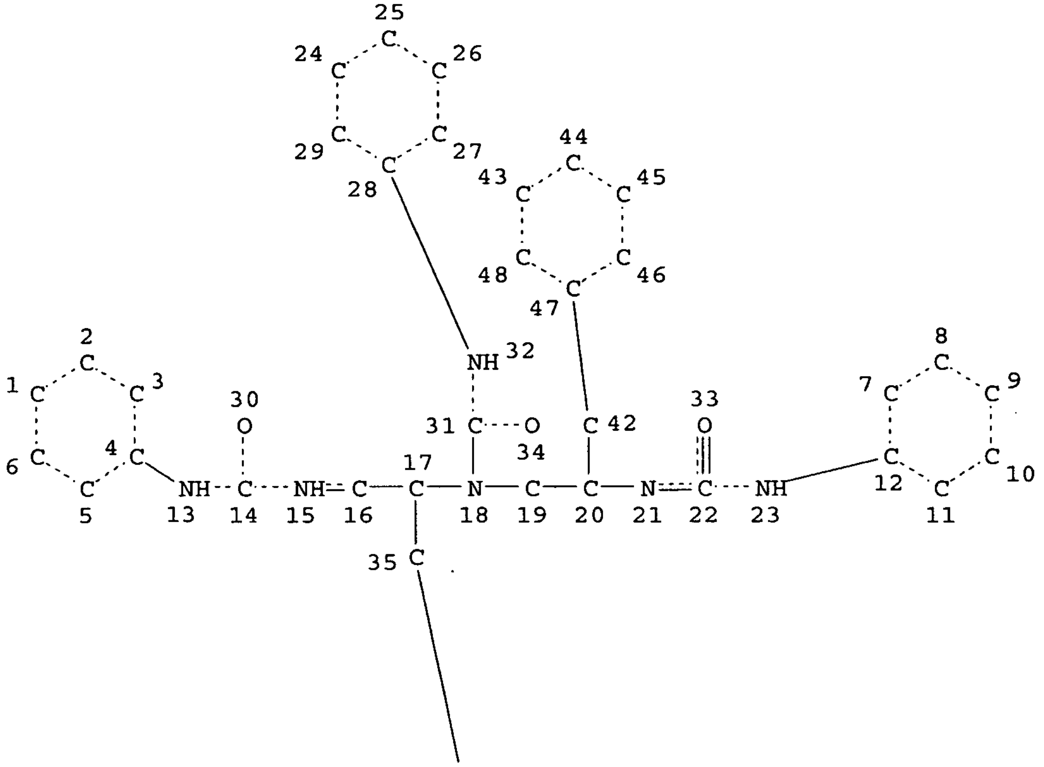
Page 3



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C 14
O 30
NH 15
C 16
C 17
N 18
C 19
C 20
N 21
C 22
O 33
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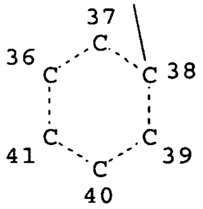
C 31
O 34
NH 32
C 42
C 35

Page 1-A



Page 2-A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

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L7            65 SEA FILE=REGISTRY SUB=L5 SSS FUL L6

100.0% PROCESSED      65 ITERATIONS                        65 ANSWERS
SEARCH TIME: 00.00.01
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COST IN U.S. DOLLARS                                 SINCE FILE      TOTAL
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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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                                                   ENTRY    SESSION
FULL ESTIMATED COST                                252.78     252.99

FILE 'MEDLINE' ENTERED AT 14:27:29 ON 08 AUG 2006

FILE 'BIOSIS' ENTERED AT 14:27:29 ON 08 AUG 2006
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FILE 'EMBASE' ENTERED AT 14:27:29 ON 08 AUG 2006
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FILE 'CAPLUS' ENTERED AT 14:27:29 ON 08 AUG 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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L8             0 FILE MEDLINE
L9             0 FILE BIOSIS
L10            0 FILE EMBASE
L11            3 FILE CAPLUS

TOTAL FOR ALL FILES
L12            3 L7

=> d 1-3 ibib abs hitstr

L12  ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:474920  CAPLUS
DOCUMENT NUMBER:          143:19969
TITLE:                    Peptidyl and nonpeptidyl compounds for derepression of
                          IAP-inhibited caspase and therapeutic and drug
                          screening uses
INVENTOR(S):              Reed, John C.; Houghten, Richard A.; Nefzi, Adel;
                          Ostresh, John M.; Pinilla, Clemencia; Welsh, Kate
PATENT ASSIGNEE(S):       The Burnham Institute, USA; Torrey Pines Institute for
                          Molecular Studies
SOURCE:                   U.S. Pat. Appl. Publ., 182 pp., Cont.-in-part of U.S.
                          Ser. No. 302,811.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.          KIND    DATE          APPLICATION NO.         DATE
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     US 2005119176        A1     20050602      US 2003-748128          20031224
     US 2003180805        A1     20030925      US 2002-302811          20021121
     US 6911426           B2     20050628
     US 2005159359        A1     20050721      US 2004-21517           20041223
PRIORITY APPLN. INFO.:                         US 2001-331957P      P  20011121
                                               US 2002-302811      A2  20021121
AB   The invention provides isolated agents having a core peptidyl or
     nonpeptidyl (e.g., urea derivative, diketopiperazine derivative) structure,
     wherein the agent derepresses an IAP-inhibited caspase.  The invention
     also provides a method of derepressing an IAP-inhibited caspase.  The
     method consists of contacting an IAP-inhibited caspase with an effective
     amount of an agent to derepress an IAP-inhibited caspase.  The methods of
     the invention can be used for promoting apoptosis in a cell and for
```

Ø
APP

APP

reducing the severity of a pathol. (e.g., cancer) characterized by reduced levels of apoptosis. Methods for identifying agents that derepress an IAP-inhibited caspase are also provided.

```
IT   295343-36-1 295343-40-7 537051-01-7
     537051-02-8 537051-03-9 537051-04-0
     537051-05-1 537051-07-3 537051-08-4
     537051-09-5 537051-10-8 537051-12-0
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     537051-16-4 537051-17-5 537051-18-6
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     537052-92-9 537052-93-0 537052-94-1
     537052-95-2 537052-96-3 537052-97-4
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     537053-04-6 537053-05-7 537053-06-8
     540529-33-7 540529-35-9 540529-37-1
     852819-25-1 852819-28-4 852819-29-5
     852819-41-1
     RL: BSU (Biological study, unclassified); CST (Combinatorial study,
     unclassified); PAC (Pharmacological activity); BIOL (Biological study);
     CMBI (Combinatorial study)
        (peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited
        caspase and therapeutic and drug screening uses)
RN   295343-36-1  CAPLUS
CN   Urea, N-[(2S)-2-[(cycloheptylmethyl)[(phenylamino)carbonyl]amino]-3-
     phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-
     (phenylmethyl)ethyl]- (9CI)  (CA INDEX NAME)
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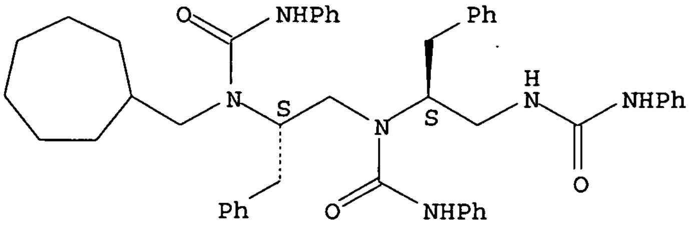
Absolute stereochemistry.



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RN   295343-40-7  CAPLUS
CN   Urea, N-[(2S)-2-[[3-(4-methylphenyl)propyl][(phenylamino)carbonyl]amino]-3-
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     (phenylmethyl)ethyl]- (9CI)  (CA INDEX NAME)
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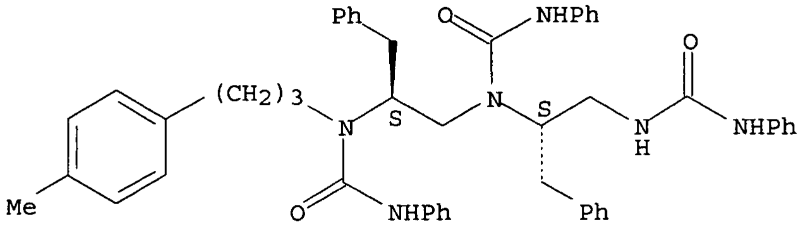
Absolute stereochemistry.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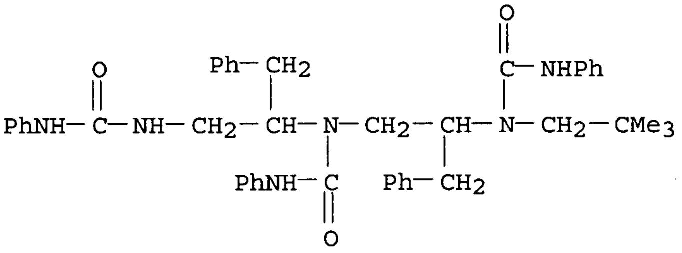
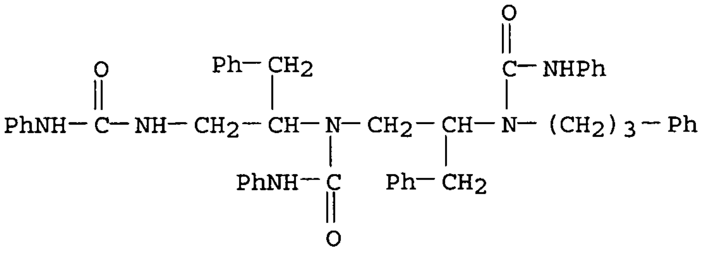
O
NHPh
O
(CH2)3
N
S
N
S
N
H
NHPh
Me
O
NHPh
Ph

RN 537051-01-7 CAPLUS
CN Urea, N-[2-[(2,2-dimethylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


O
C— NHPh
O
Ph— CH2
PhNH— C— NH— CH2— CH— N— CH2— CH— N— CH2— CMe3
PhNH— C
Ph— CH2
O

RN 537051-02-8 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](3-phenylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)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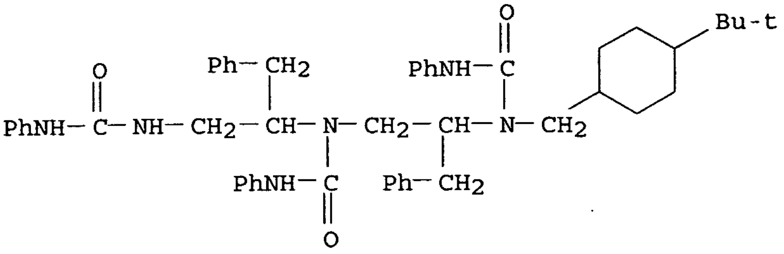
C— NHPh
O
Ph— CH2
PhNH— C— NH— CH2— CH— N— CH2— CH— N— (CH2)3— Ph
PhNH— C
Ph— CH2
O

RN 537051-03-9 CAPLUS
CN Urea, N-[2-[[[4-(1,1-dimethylethyl)cyclohexyl]methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)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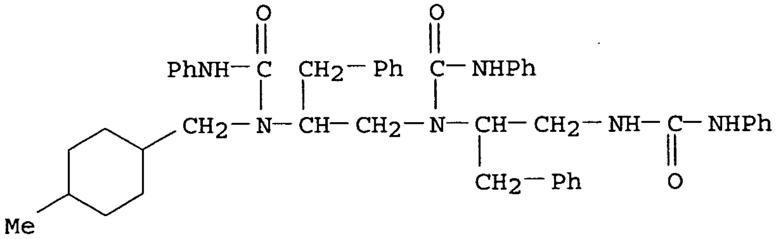
O
NH
CH2
CH
N
Ph
PhNH
Bu-t

RN 537051-04-0 CAPLUS
CN Urea, N-[2-[[(4-methylcyclohexyl)methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)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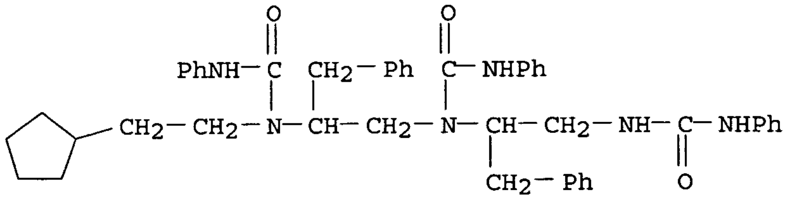
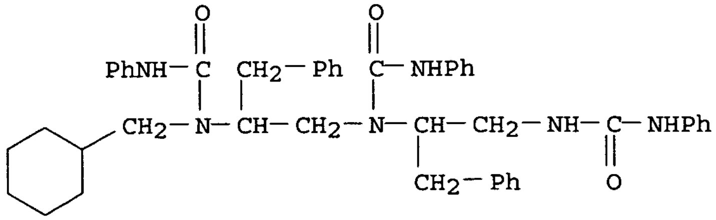
CH2
Ph
NHPh
N
CH
NH
Me
O

RN 537051-05-1 CAPLUS
CN Urea, N-[2-[(2-cyclopentylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


PhNH
CH2
Ph
NHPh
N
CH
NH
O

RN 537051-07-3 CAPLUS
CN Urea, N-[2-[(cyclohexylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)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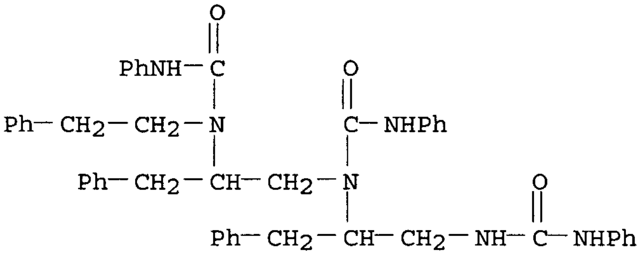
CH2
Ph
NHPh
N
CH
NH
O

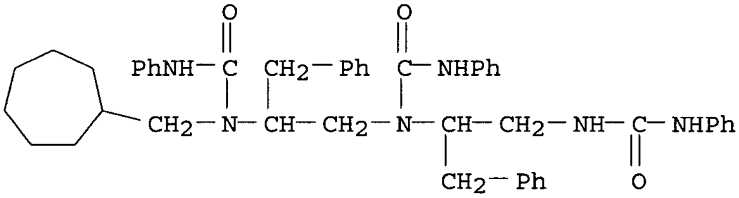
RN 537051-08-4 CAPLUS

CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](2-phenylethyl)amino]propyl]- (9CI) (CA INDEX NAME)


PhNH—C
O
Ph—CH2—CH2—N
Ph—CH2—CH—CH2—N
C—NHPh
O
Ph—CH2—CH—CH2—NH—C—NHPh
O

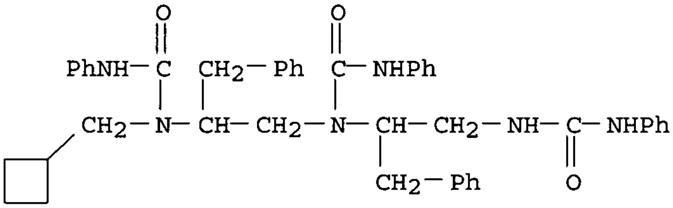
RN 537051-09-5 CAPLUS

CN Urea, N-[2-[(cycloheptylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


O
PhNH—C
CH2—Ph
O
C—NHPh
CH2—N—CH—CH2—N—CH—CH2—NH—C—NHPh
CH2—Ph
O

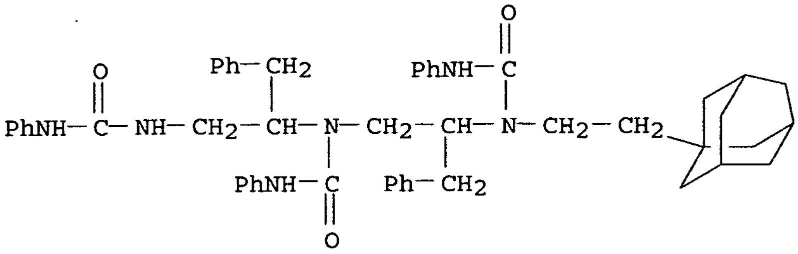
RN 537051-10-8 CAPLUS

CN Urea, N-[2-[(cyclobutylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


O
PhNH—C
CH2—Ph
O
C—NHPh
CH2—N—CH—CH2—N—CH—CH2—NH—C—NHPh
CH2—Ph
O

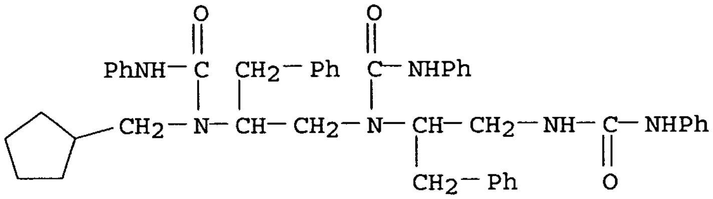
RN 537051-12-0 CAPLUS

CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](2-tricyclo[3.3.1.13,7]dec-1-ylethyl)amino]propyl]- (9CI) (CA INDEX NAME)



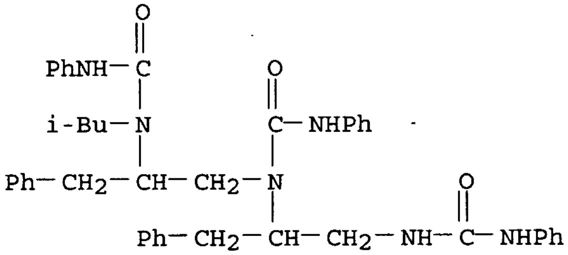
RN 537051-13-1 CAPLUS

CN Urea, N-[2-[(cyclopentylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



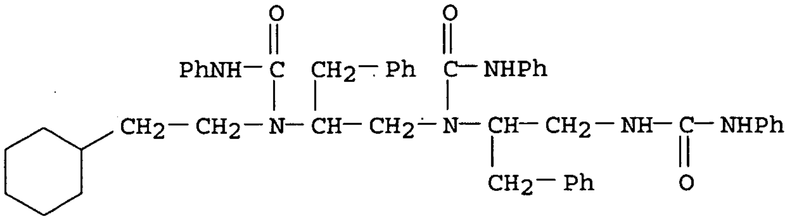
RN 537051-14-2 CAPLUS

CN Urea, N-[2-[(2-methylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

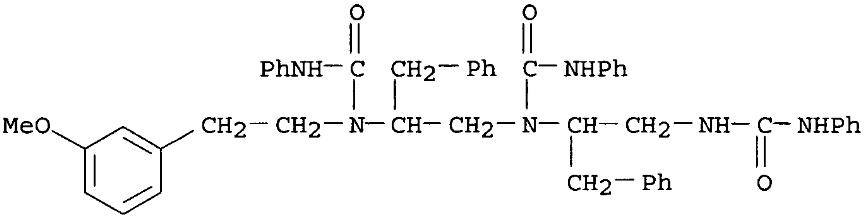


RN 537051-15-3 CAPLUS

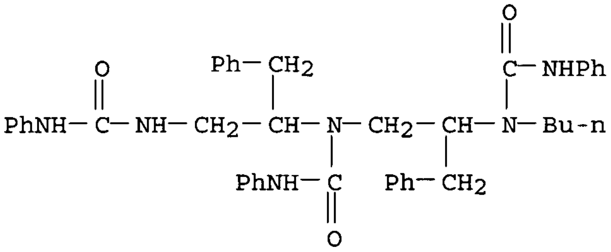
CN Urea, N-[2-[(2-cyclohexylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



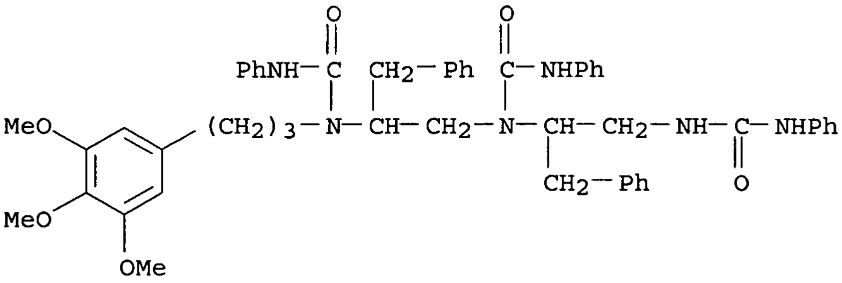
RN 537051-16-4 CAPLUS
CN Urea, N-[2-[[2-(3-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



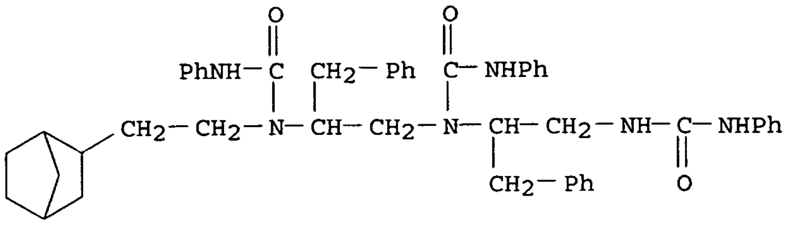
RN 537051-17-5 CAPLUS
CN Urea, N-[2-[butyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 537051-18-6 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl][3-(3,4,5-trimethoxyphenyl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

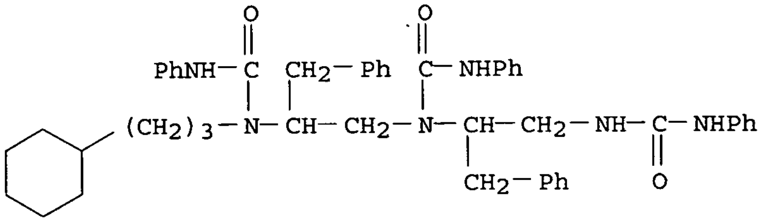


RN 537051-20-0 CAPLUS
CN Urea, N-[2-[(2-bicyclo[2.2.1]hept-2-ylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



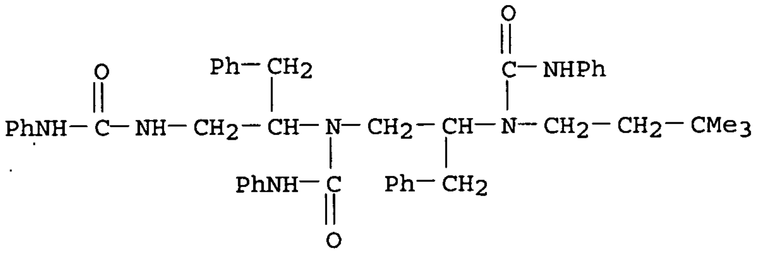
PhNH
CH2 Ph
NHPh
CH2 CH2 N CH CH2 N CH CH2 NH C NHPh
CH2 Ph

RN 537051-21-1 CAPLUS
CN Urea, N-[2-[(3-cyclohexylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



PhNH
CH2 Ph
NHPh
(CH2)3 N CH CH2 N CH CH2 NH C NHPh
CH2 Ph

RN 537051-22-2 CAPLUS
CN Urea, N-[2-[(3,3-dimethylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



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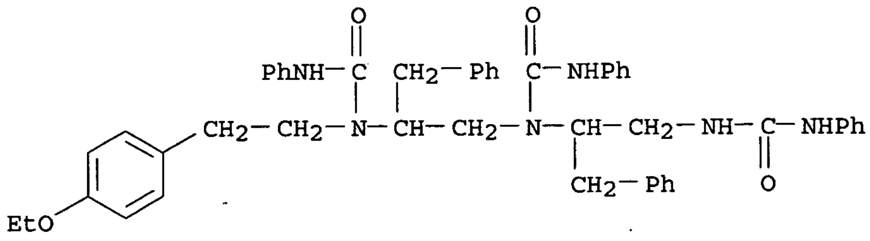
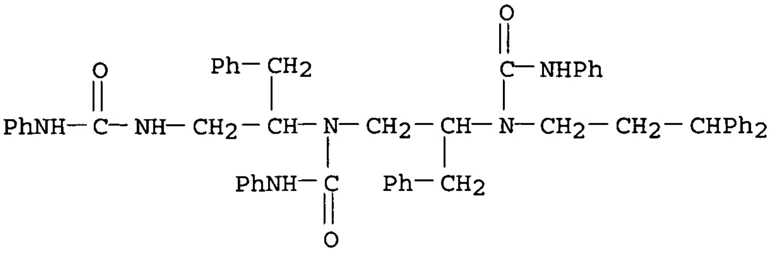
NHPh
PhNH C NH CH2 CH N CH2 CH N CH2 CH2 CMe3
PhNH
Ph CH2

RN 537051-23-3 CAPLUS
CN Urea, N-[2-[[2-(4-ethoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



PhNH
CH2 Ph
NHPh
CH2 CH2 N CH CH2 N CH CH2 NH C NHPh
CH2 Ph
EtO

RN 537051-24-4 CAPLUS
CN Urea, N-[2-[(3,3-diphenylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



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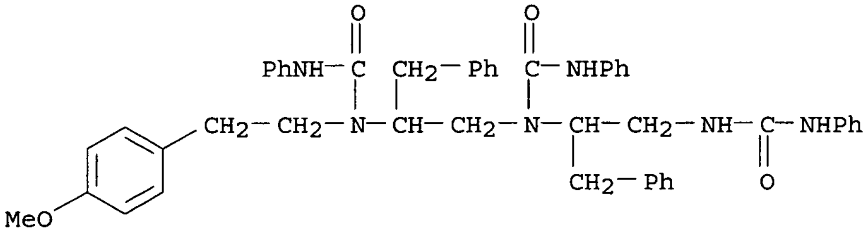
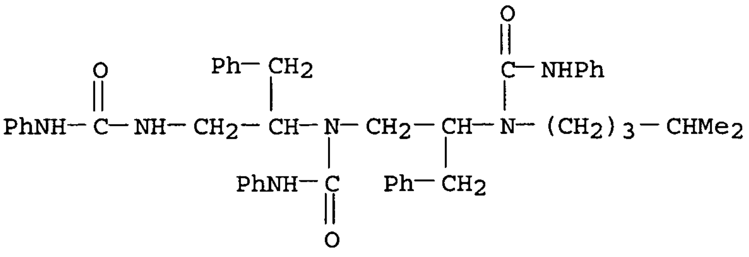
RN 537051-25-5 CAPLUS
CN Urea, N-[2-[[2-(4-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

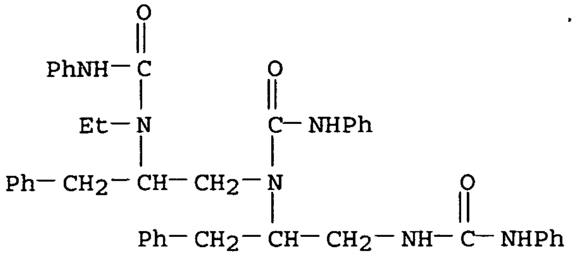


RN 537051-26-6 CAPLUS
CN Urea, N-[2-[(4-methylpentyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

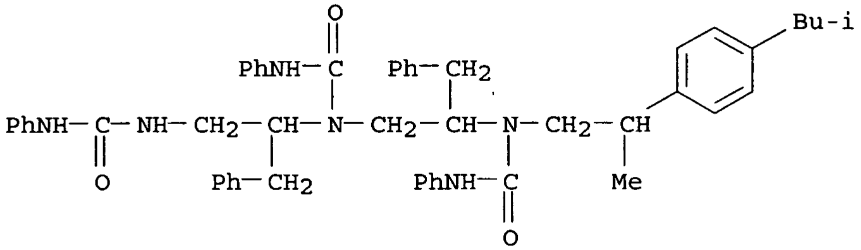


$$\mathrm{PhNH-\overset{O}{\overset{\|}{C}}-NH-CH_2-\overset{Ph-CH_2}{\overset{|}{CH}}-\underset{\underset{O}{\underset{\|}{PhNH-C}}}{\underset{|}{N}}-CH_2-\underset{Ph-CH_2}{\underset{|}{CH}}-\overset{\overset{O}{\overset{\|}{C-NHPh}}}{\overset{|}{N}}-(CH_2)_3-CHMe_2}$$

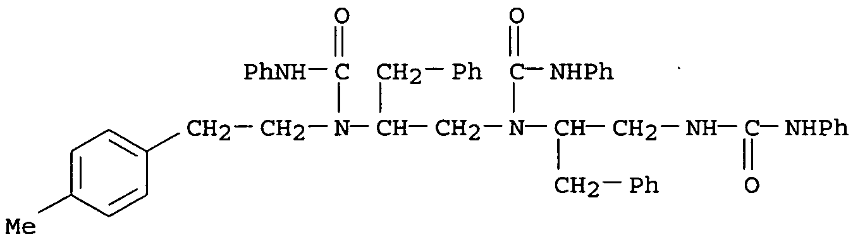
RN 537051-27-7 CAPLUS
CN Urea, N-[2-[ethyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 537051-28-8 CAPLUS
CN Urea, N-[2-[[2-[4-(2-methylpropyl)phenyl]propyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

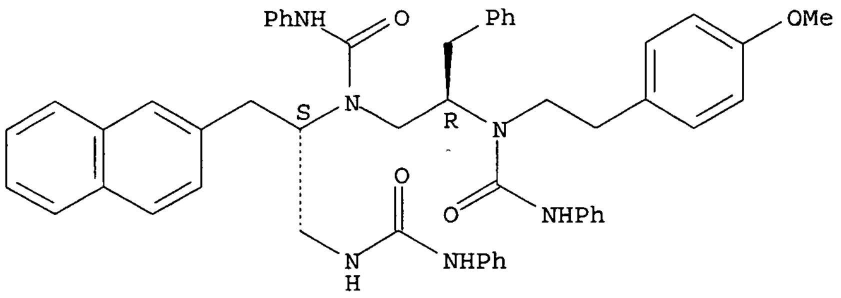


RN 537051-29-9 CAPLUS
CN Urea, N-[2-[[2-(4-methylphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 537052-67-8 CAPLUS
CN Urea, N-[(2R)-2-[[2-(4-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N-[(1S)-1-(2-naphthalenylmethyl)-2-[[(phenylamino)carbonyl]amino]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

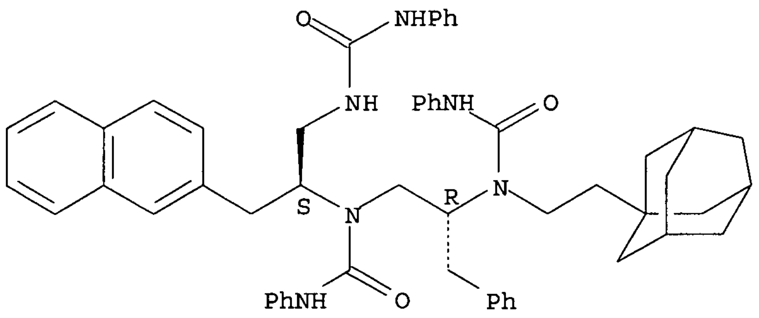
Absolute stereochemistry.



RN 537052-68-9 CAPLUS

CN Urea, N-[(1S)-1-(2-naphthalenylmethyl)-2-[[(phenylamino)carbonyl]amino]ethyl]-N'-phenyl-N-[(2R)-3-phenyl-2-[[(phenylamino)carbonyl](2-tricyclo[3.3.1.13,7]dec-1-ylethyl)amino]propyl]- (9CI) (CA INDEX NAME)

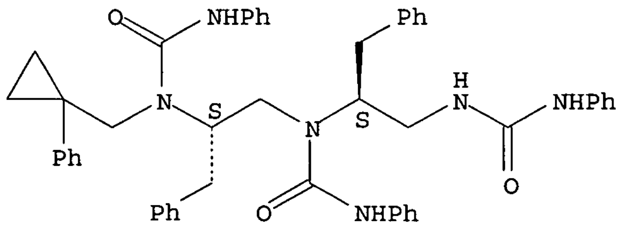
Absolute stereochemistry.



RN 537052-83-8 CAPLUS

CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl][(1-phenylcyclopropyl)methyl]amino]propyl]- (9CI) (CA INDEX NAME)

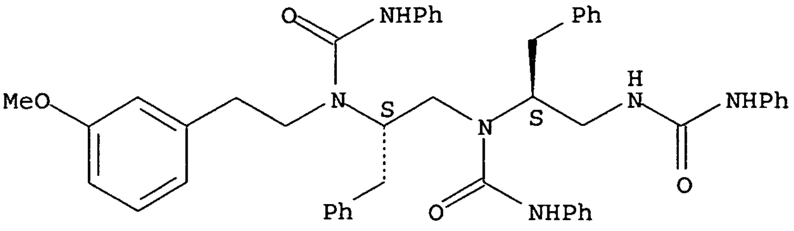
Absolute stereochemistry.



RN 537052-84-9 CAPLUS

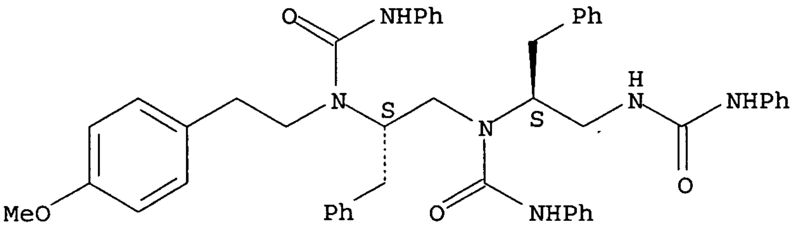
CN Urea, N-[(2S)-2-[[2-(3-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


NHPh
Ph
MeO
N
S
N
S
H
N
NHPh
O
Ph
O
NHPh
O

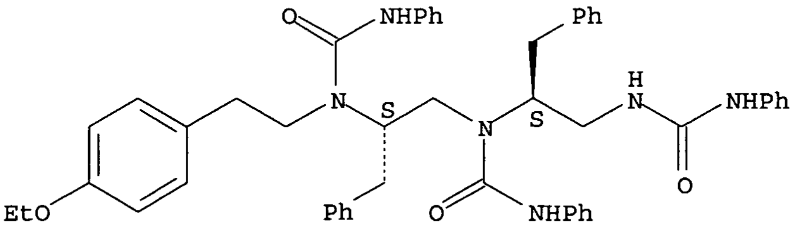
RN 537052-85-0 CAPLUS
CN Urea, N-[(2S)-2-[[2-(4-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


O
NHPh
Ph
N
S
N
S
H
N
NHPh
O
MeO
Ph
O
NHPh

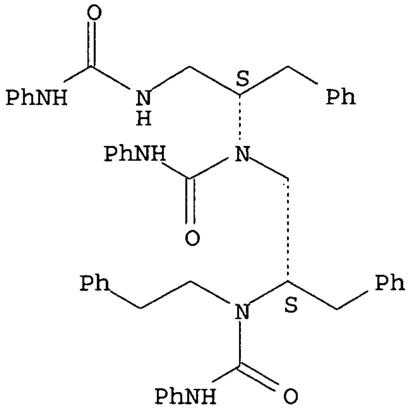
RN 537052-86-1 CAPLUS
CN Urea, N-[(2S)-2-[[2-(4-ethoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


O
NHPh
Ph
N
S
N
S
H
N
NHPh
O
EtO
Ph
O
NHPh

RN 537052-87-2 CAPLUS
CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl](2-phenylethyl)amino]propyl]- (9CI) (CA INDEX NAME)

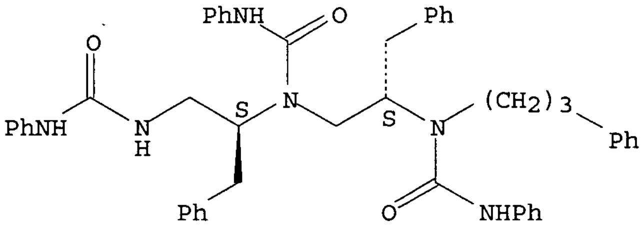
Absolute stereochemistry.



RN 537052-88-3 CAPLUS

CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl](3-phenylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)

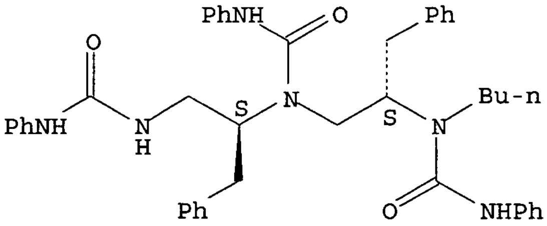
Absolute stereochemistry.



RN 537052-89-4 CAPLUS

CN Urea, N-[(2S)-2-[butyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

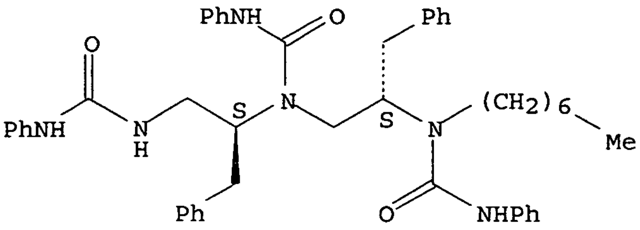
Absolute stereochemistry.



RN 537052-90-7 CAPLUS

CN Urea, N-[(2S)-2-[heptyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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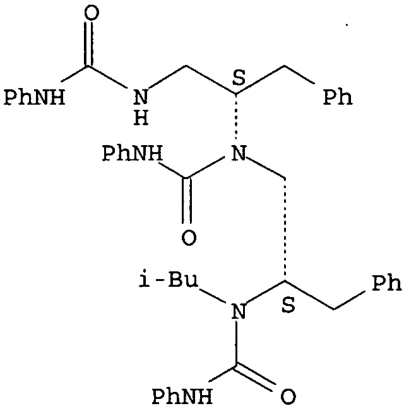
O
PhNH
O
Ph
N
H
S
N
S
N
(CH2)6
Me
Ph
O
NHPh

RN 537052-91-8 CAPLUS
CN Urea, N-[(2S)-2-[(2-methylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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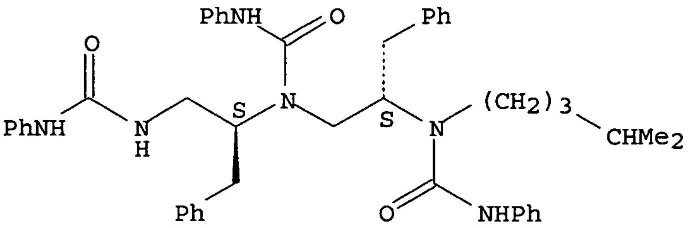
PhNH
N
H
S
Ph
PhNH
N
O
i-Bu
N
S
Ph
PhNH
O

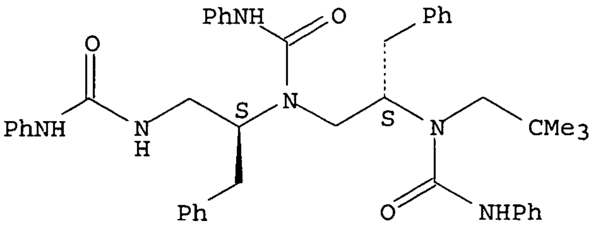
RN 537052-92-9 CAPLUS
CN Urea, N-[(2S)-2-[(4-methylpentyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


PhNH
O
PhNH
O
Ph
N
H
S
N
S
N
(CH2)3
CHMe2
Ph
O
NHPh

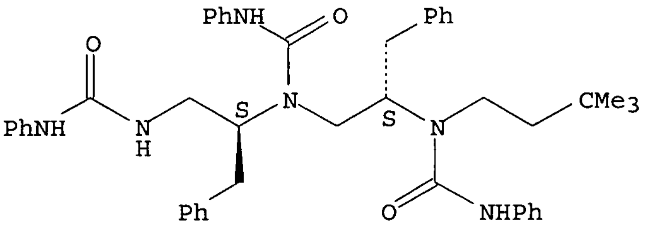
RN 537052-93-0 CAPLUS
CN Urea, N-[(2S)-2-[(2,2-dimethylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



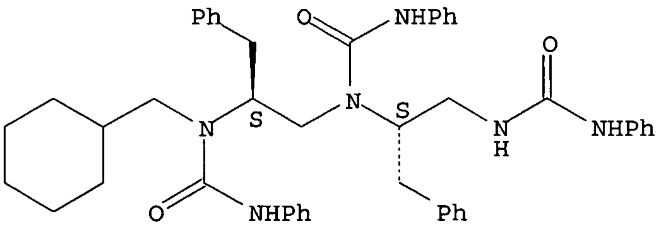
RN 537052-94-1 CAPLUS
CN Urea, N-[(2S)-2-[(3,3-dimethylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



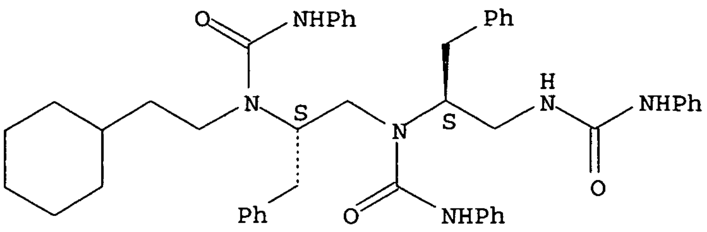
RN 537052-95-2 CAPLUS
CN Urea, N-[(2S)-2-[(cyclohexylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



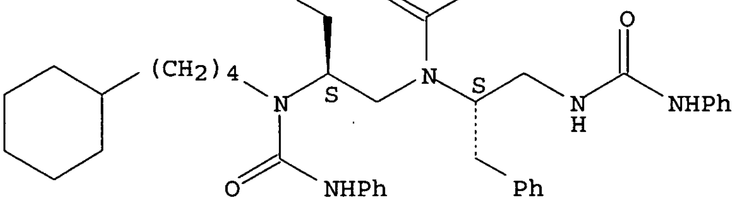
RN 537052-96-3 CAPLUS
CN Urea, N-[(2S)-2-[(2-cyclohexylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



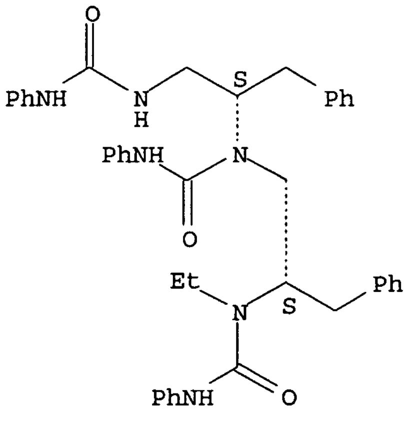
RN 537052-97-4 CAPLUS
CN Urea, N-[(2S)-2-[(4-cyclohexylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



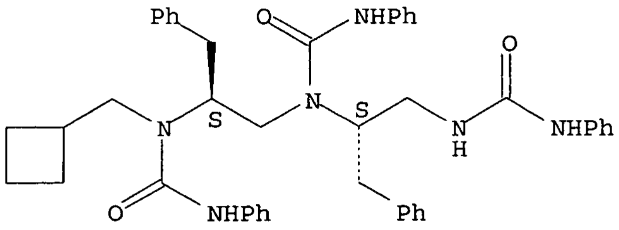
RN 537052-98-5 CAPLUS
CN Urea, N-[(2S)-2-[ethyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537052-99-6 CAPLUS
CN Urea, N-[(2S)-2-[(cyclobutylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

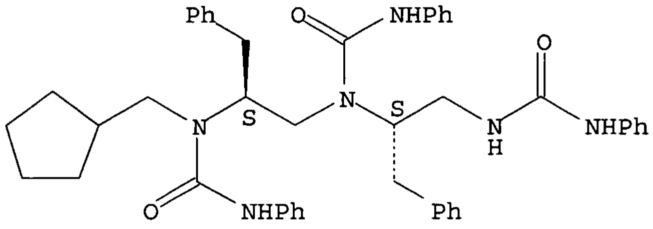
Absolute stereochemistry.



RN 537053-00-2 CAPLUS

CN Urea, N-[(2S)-2-[(cyclopentylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

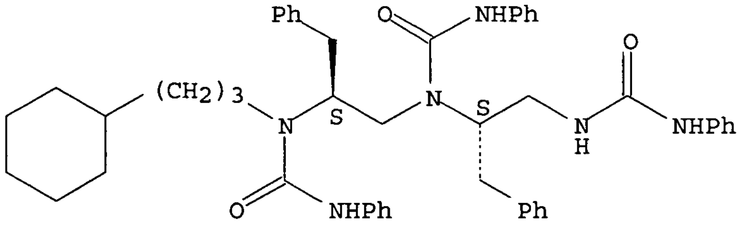
Absolute stereochemistry.



RN 537053-01-3 CAPLUS

CN Urea, N-[(2S)-2-[(3-cyclohexylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

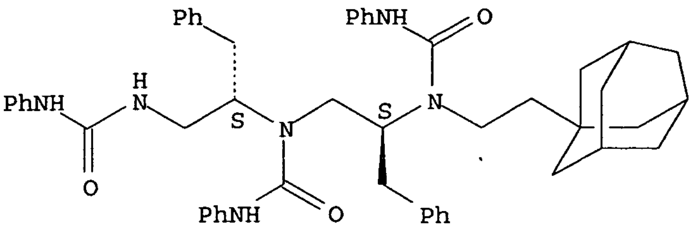
Absolute stereochemistry.



RN 537053-02-4 CAPLUS

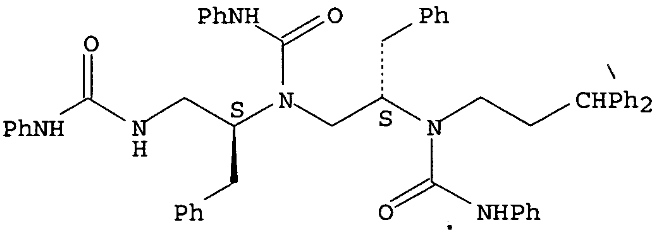
CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl](2-tricyclo[3.3.1.13,7]dec-1-ylethyl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



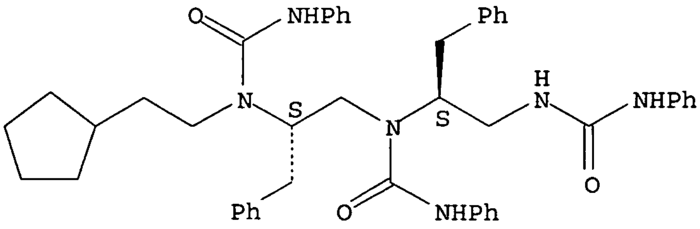
RN 537053-03-5 CAPLUS
CN Urea, N-[(2S)-2-[(3,3-diphenylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



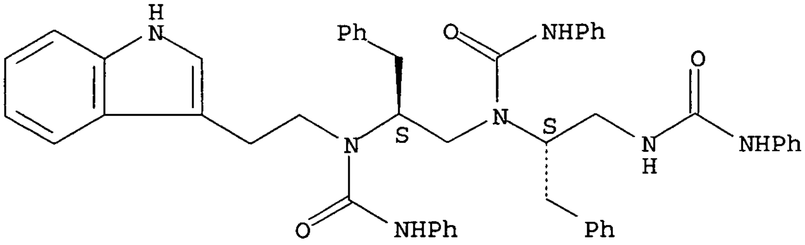
RN 537053-04-6 CAPLUS
CN Urea, N-[(2S)-2-[(2-cyclopentylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



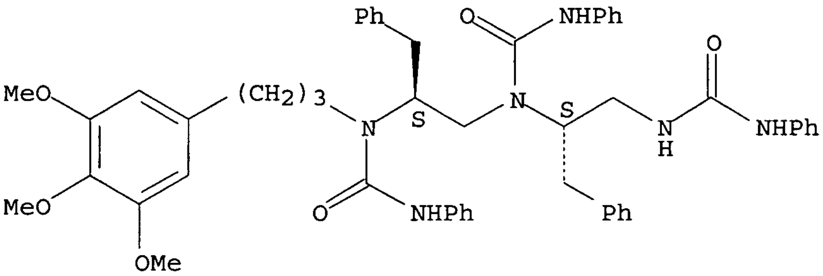
RN 537053-05-7 CAPLUS
CN Urea, N-[(2S)-2-[[2-(1H-indol-3-yl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


H
N
Ph
O
NHPh
O
N
S
N
S
N
H
NHPh
O
NHPh
Ph

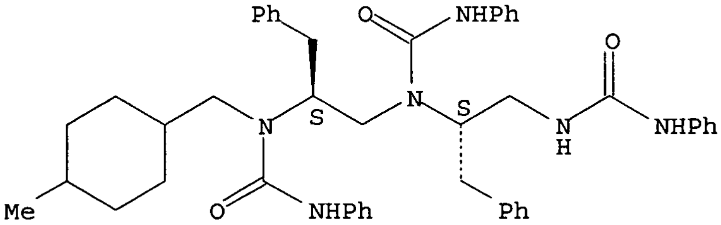
RN 537053-06-8 CAPLUS
CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl][3-(3,4,5-trimethoxyphenyl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


Ph
O
NHPh
O
MeO
(CH2)3
N
S
N
S
N
H
NHPh
MeO
O
NHPh
Ph
OMe

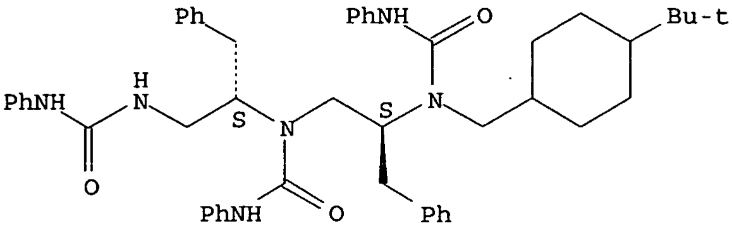
RN 540529-33-7 CAPLUS
CN Urea, N-[(2S)-2-[[(4-methylcyclohexyl)methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


Ph
O
NHPh
O
N
S
N
S
N
H
NHPh
Me
O
NHPh
Ph

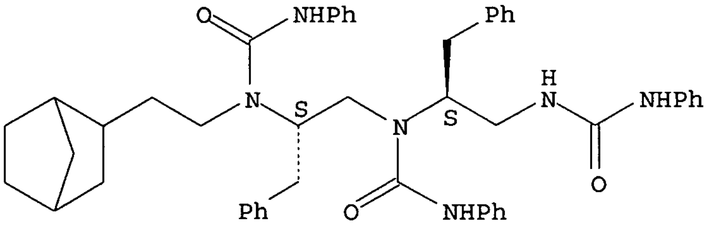
RN 540529-35-9 CAPLUS
CN Urea, N-[(2S)-2-[[[4-(1,1-dimethylethyl)cyclohexyl]methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

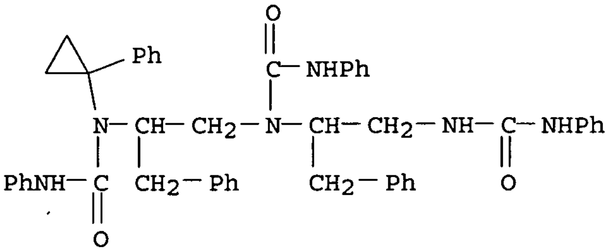


RN 540529-37-1 CAPLUS
CN Urea, N-[(2S)-2-[(2-bicyclo[2.2.1]hept-2-ylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

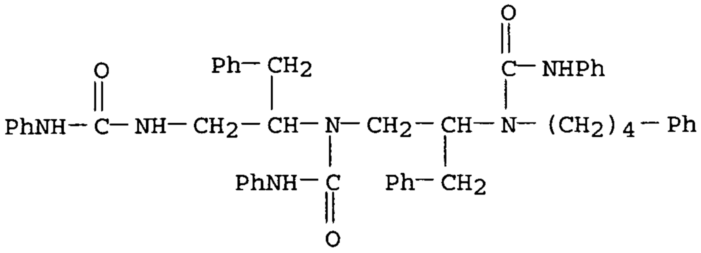
Absolute stereochemistry.



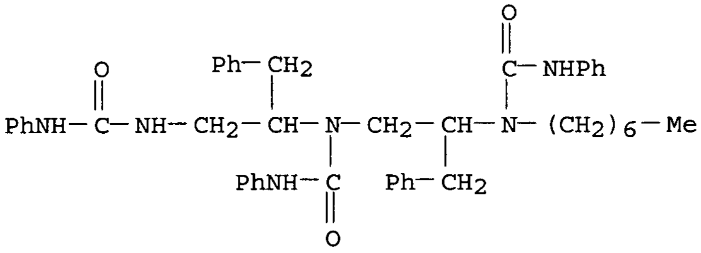
RN 852819-25-1 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](1-phenylcyclopropyl)amino]propyl]- (9CI) (CA INDEX NAME)



RN 852819-28-4 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](4-phenylbutyl)amino]propyl]- (9CI) (CA INDEX NAME)

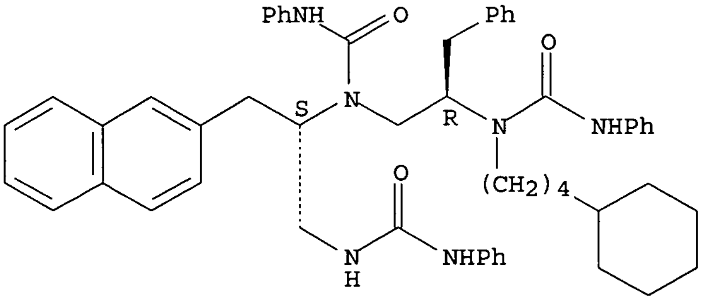


RN 852819-29-5 CAPLUS
CN Urea, N-[2-[heptyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 852819-41-1 CAPLUS
CN Urea, N-[(2R)-2-[(4-cyclohexylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N-[(1S)-1-(2-naphthalenylmethyl)-2-[[(phenylamino)carbonyl]amino]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2003:434582 CAPLUS
DOCUMENT NUMBER:	139:30774
TITLE:	Methods and compositions using peptidyl and nonpeptidyl compounds for derepression of IAP-inhibited caspase, therapeutic use, and methods for identification of agents
INVENTOR(S):	Reed, John C.; Houghten, Richard A.; Nefzi, Adel; Ostresh, John M.; Pinilla, Clemencia; Welsh, Kate
PATENT ASSIGNEE(S):	The Burnham Institute, USA; Torrey Pines Institute for

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                           Molecular Studies
SOURCE:                    PCT Int. Appl., 182 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:    2
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.       DATE
     ---------------     ----   --------   --------------------  --------
     WO 2003045974        A2    20030605   WO 2002-US37577       20021121
     WO 2003045974        A3    20040219
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2467892           AA    20030605   CA 2002-2467892       20021121
     AU 2002359457        A1    20030610   AU 2002-359457        20021121
     AU 2002359457        A2    20030610
     EP 1465649           A2    20041013   EP 2002-793997        20021121
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     JP 2005510569        T2    20050421   JP 2003-547423        20021121
     CN 1615148           A     20050511   CN 2002-827412        20021121
PRIORITY APPLN. INFO.:                     US 2001-331957P    P  20011121
                                           WO 2002-US37577    W  20021121
AB   The invention provides isolated agents having a core peptidyl or
     nonpeptidyl (e.g. urea derivative, diketopiperazine derivative) structure,
wherein
     the agent derepresses an IAP-inhibited caspase.  The invention also
     provides a method of derepressing an IAP-inhibited caspase.  The method
     consists of contacting an IAP-inhibited caspase with an effective amount of
     an agent to derepress an IAP-inhibited caspase.  The methods of the
     invention can be used for promoting apoptosis in a cell and for reducing
     the severity of a pathol. (e.g. cancer) characterized by reduced levels of
     apoptosis.  Methods for identifying agents that derepress an IAP-inhibited
     caspase are also provided.
IT   295343-36-1 295343-40-7 537051-01-7
     537051-02-8 537051-03-9 537051-04-0
     537051-05-1 537051-06-2 537051-07-3
     537051-08-4 537051-09-5 537051-10-8
     537051-11-9 537051-12-0 537051-13-1
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     537051-17-5 537051-18-6 537051-19-7
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     537051-29-9 537052-67-8 537052-68-9
     537052-69-0 537052-83-8 537052-84-9
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     537053-03-5 537053-04-6 537053-05-7
     537053-06-8 540529-33-7 540529-35-9 54052
     9-37-1
     RL: CST (Combinatorial study, unclassified); PAC (Pharmacological
     activity); THU (Therapeutic use); BIOL (Biological study); CMBI
     (Combinatorial study); USES (Uses)
        (peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited
        caspase, therapeutic use, and methods for identification of agents)
RN   295343-36-1  CAPLUS
CN   Urea, N-[(2S)-2-[(cycloheptylmethyl)[(phenylamino)carbonyl]amino]-3-
     phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-
     (phenylmethyl)ethyl]- (9CI)  (CA INDEX NAME)

Absolute stereochemistry.
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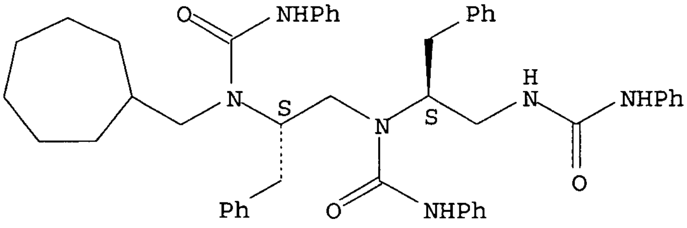

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RN   295343-40-7  CAPLUS
CN   Urea, N-[(2S)-2-[[3-(4-methylphenyl)propyl][(phenylamino)carbonyl]amino]-3-
     phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-
     (phenylmethyl)ethyl]- (9CI)  (CA INDEX NAME)

Absolute stereochemistry.
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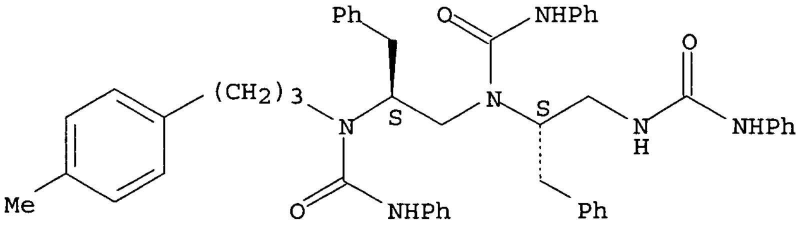

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RN   537051-01-7  CAPLUS
CN   Urea, N-[2-[(2,2-dimethylpropyl)[(phenylamino)carbonyl]amino]-3-
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     (phenylmethyl)ethyl]- (9CI)  (CA INDEX NAME)
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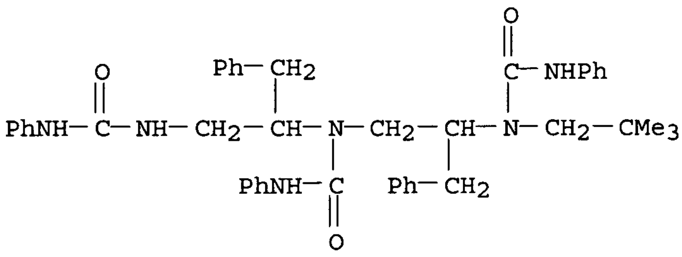
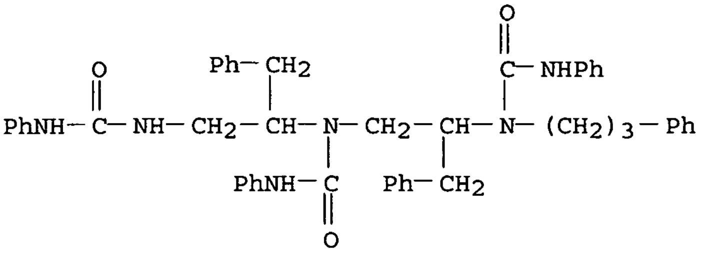
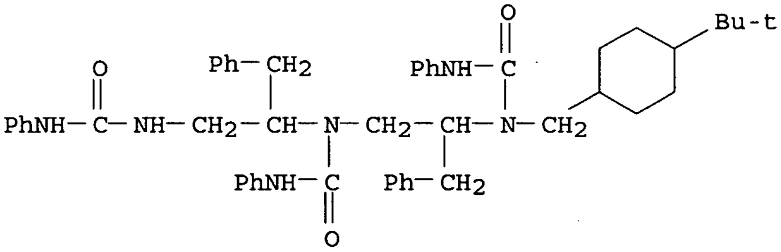


$$\mathrm{PhNH{-}\overset{O}{\overset{\|}{C}}{-}NH{-}CH_2{-}\overset{Ph-CH_2}{\overset{|}{CH}}{-}\underset{\underset{O}{\underset{\|}{PhNH-C}}}{\underset{|}{N}}{-}CH_2{-}\underset{Ph-CH_2}{\underset{|}{CH}}{-}\overset{\overset{O}{\overset{\|}{C-NHPh}}}{\overset{|}{N}}{-}CH_2{-}CMe_3}$$

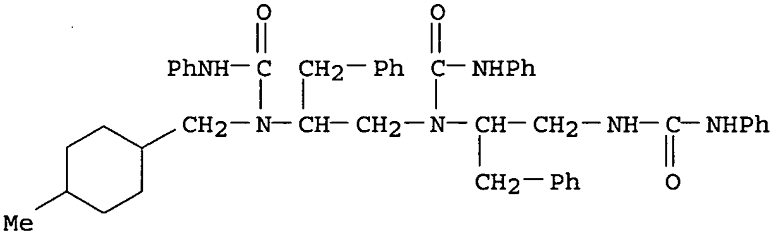
RN 537051-02-8 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](3-phenylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)



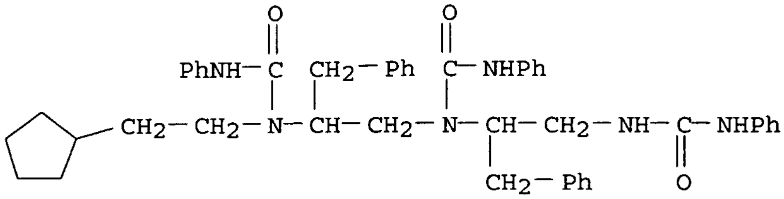
RN 537051-03-9 CAPLUS
CN Urea, N-[2-[[[4-(1,1-dimethylethyl)cyclohexyl]methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



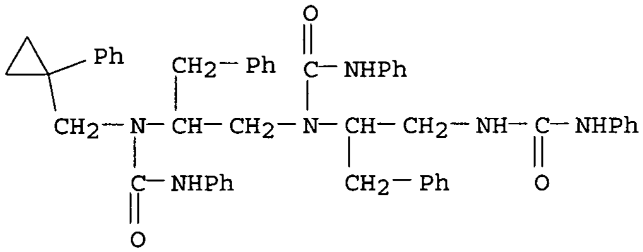
RN 537051-04-0 CAPLUS
CN Urea, N-[2-[[(4-methylcyclohexyl)methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



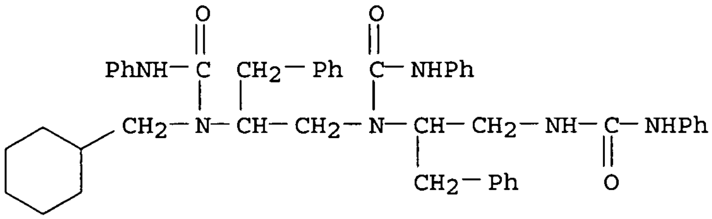
RN 537051-05-1 CAPLUS
CN Urea, N-[2-[(2-cyclopentylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



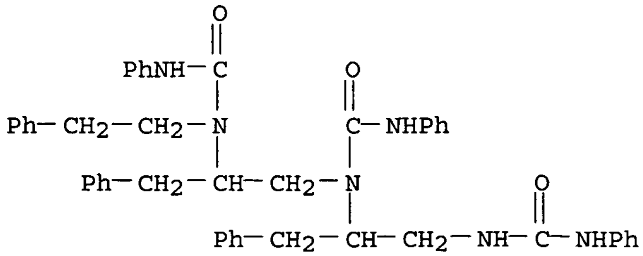
RN 537051-06-2 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl][(1-phenylcyclopropyl)methyl]amino]propyl]- (9CI) (CA INDEX NAME)



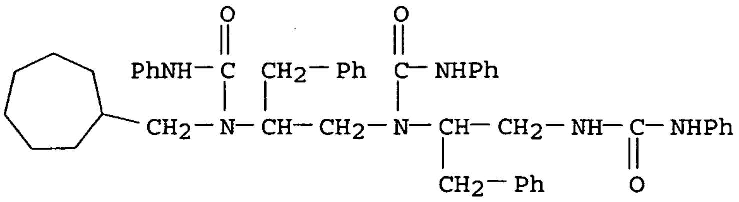
RN 537051-07-3 CAPLUS
CN Urea, N-[2-[(cyclohexylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



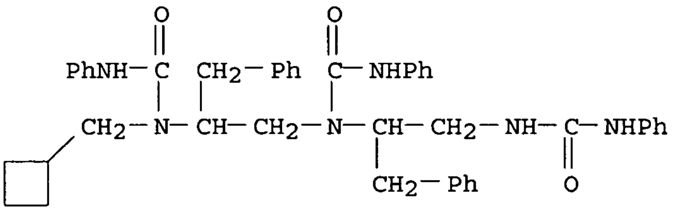
RN 537051-08-4 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](2-phenylethyl)amino]propyl]- (9CI) (CA INDEX NAME)



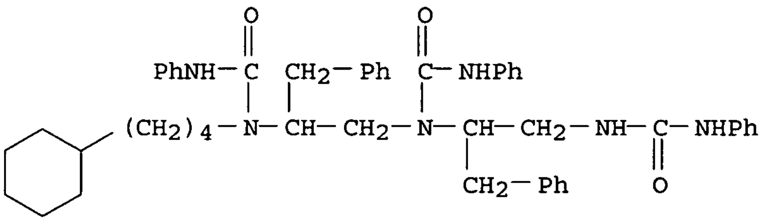
RN 537051-09-5 CAPLUS
CN Urea, N-[2-[(cycloheptylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


O
O
PhNH— C
CH2— Ph
C— NHPh
CH2— N— CH— CH2— N— CH— CH2— NH— C— NHPh
CH2— Ph
O

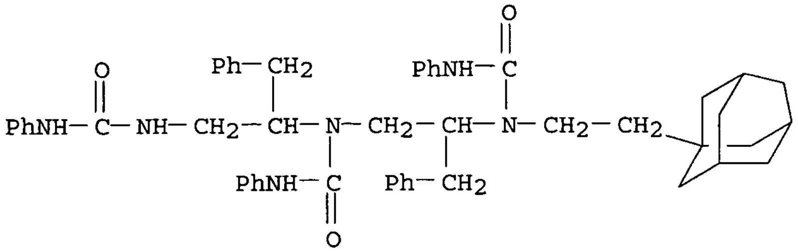
RN 537051-10-8 CAPLUS
CN Urea, N-[2-[(cyclobutylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


O
O
PhNH— C
CH2— Ph
C— NHPh
CH2— N— CH— CH2— N— CH— CH2— NH— C— NHPh
CH2— Ph
O

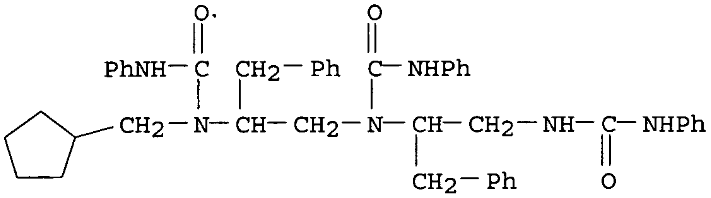
RN 537051-11-9 CAPLUS
CN Urea, N-[2-[(4-cyclohexylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)


O
O
PhNH— C
CH2— Ph
C— NHPh
(CH2) 4 — N— CH— CH2— N— CH— CH2— NH— C— NHPh
CH2— Ph
O

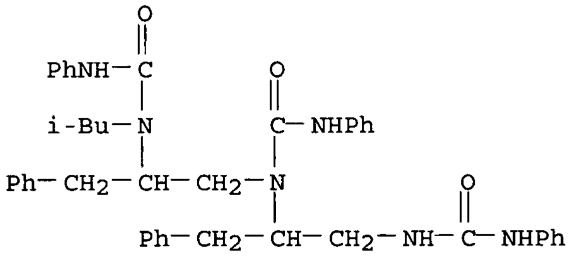
RN 537051-12-0 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl](2-tricyclo[3.3.1.13,7]dec-1-ylethyl)amino]propyl]- (9CI) (CA INDEX NAME)



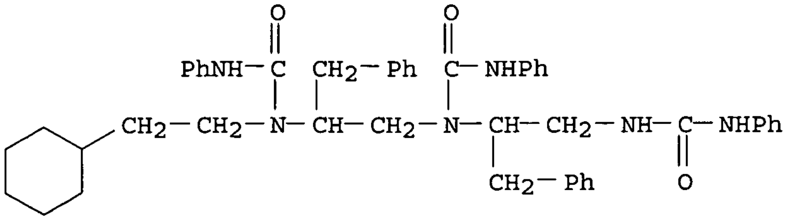
RN 537051-13-1 CAPLUS
CN Urea, N-[2-[(cyclopentylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



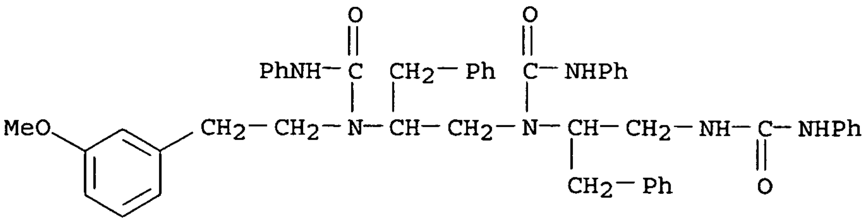
RN 537051-14-2 CAPLUS
CN Urea, N-[2-[(2-methylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



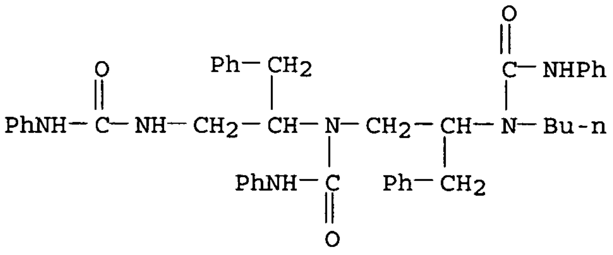
RN 537051-15-3 CAPLUS
CN Urea, N-[2-[(2-cyclohexylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



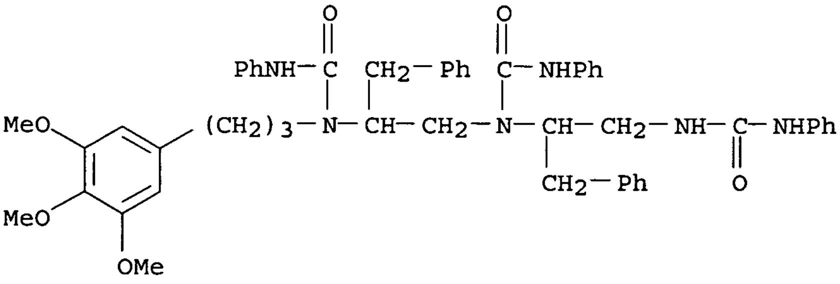
RN 537051-16-4 CAPLUS
CN Urea, N-[2-[[2-(3-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



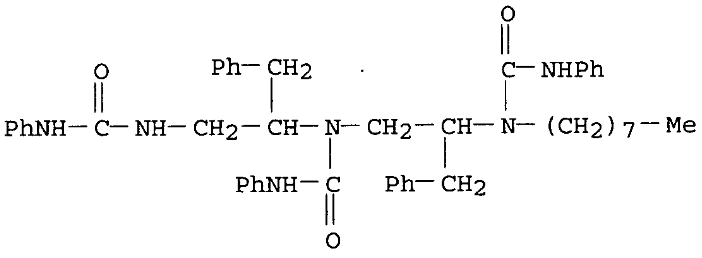
RN 537051-17-5 CAPLUS
CN Urea, N-[2-[butyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 537051-18-6 CAPLUS
CN Urea, N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[3-phenyl-2-[[(phenylamino)carbonyl][3-(3,4,5-trimethoxyphenyl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

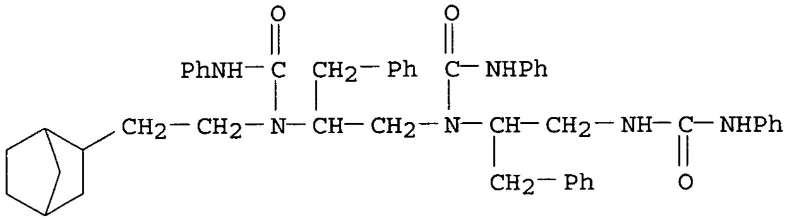


RN 537051-19-7 CAPLUS
CN Urea, N-[2-[octyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

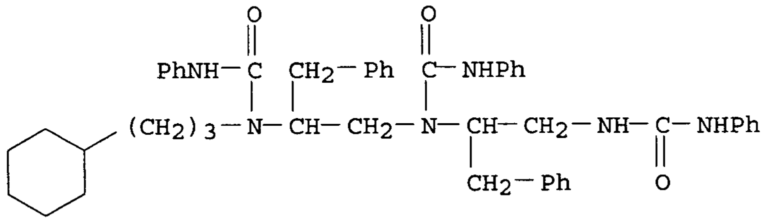


$$\mathrm{PhNH{-}C({=}O){-}NH{-}CH_2{-}CH(CH_2{-}Ph){-}N(C({=}O){-}NHPh){-}CH_2{-}CH(CH_2{-}Ph){-}N(C({=}O){-}NHPh){-}(CH_2)_7{-}Me}$$

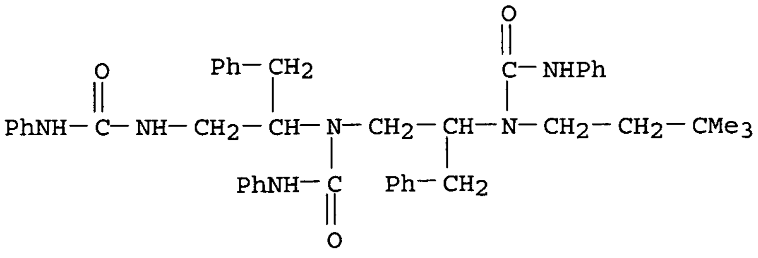
RN 537051-20-0 CAPLUS
CN Urea, N-[2-[(2-bicyclo[2.2.1]hept-2-ylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 537051-21-1 CAPLUS
CN Urea, N-[2-[(3-cyclohexylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

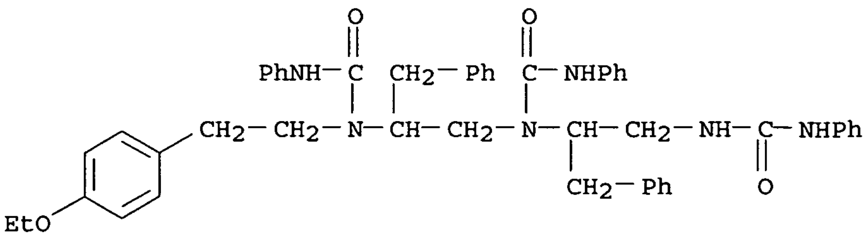


RN 537051-22-2 CAPLUS
CN Urea, N-[2-[(3,3-dimethylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

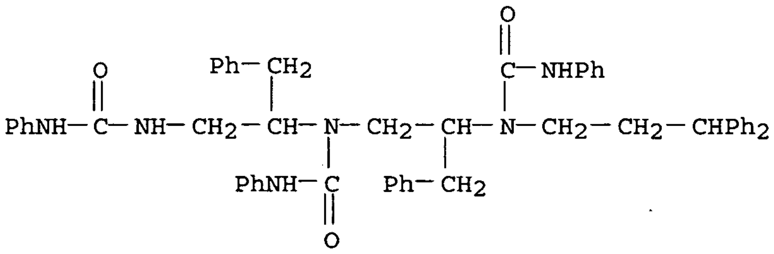


$$\mathrm{PhNH{-}C({=}O){-}NH{-}CH_2{-}CH(CH_2{-}Ph){-}N(C({=}O){-}NHPh){-}CH_2{-}CH(CH_2{-}Ph){-}N(C({=}O){-}NHPh){-}CH_2{-}CH_2{-}CMe_3}$$

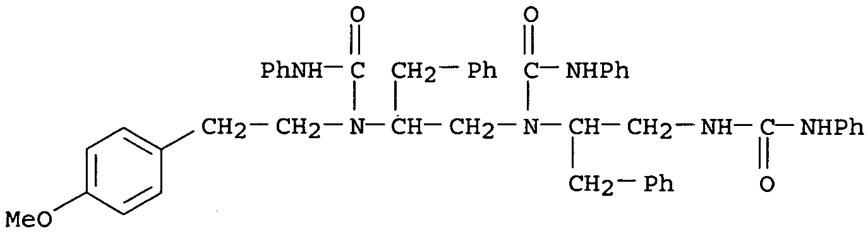
RN 537051-23-3 CAPLUS
CN Urea, N-[2-[[2-(4-ethoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



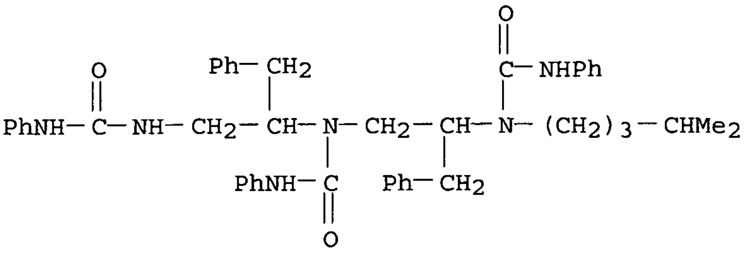
RN 537051-24-4 CAPLUS
CN Urea, N-[2-[(3,3-diphenylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



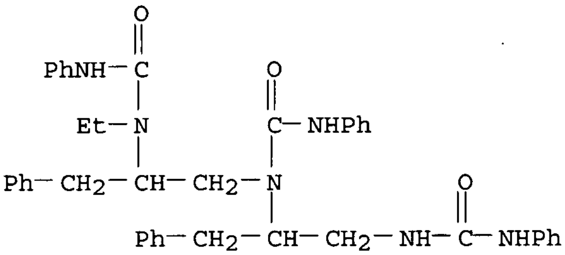
RN 537051-25-5 CAPLUS
CN Urea, N-[2-[[2-(4-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



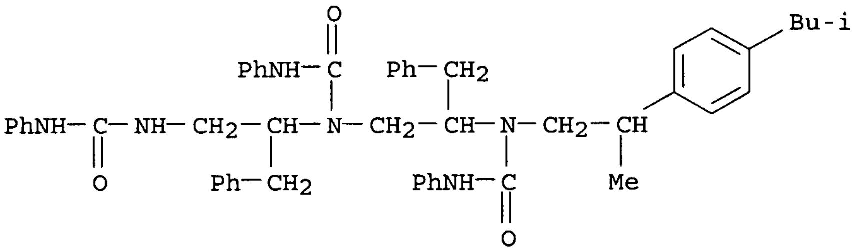
RN 537051-26-6 CAPLUS
CN Urea, N-[2-[(4-methylpentyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



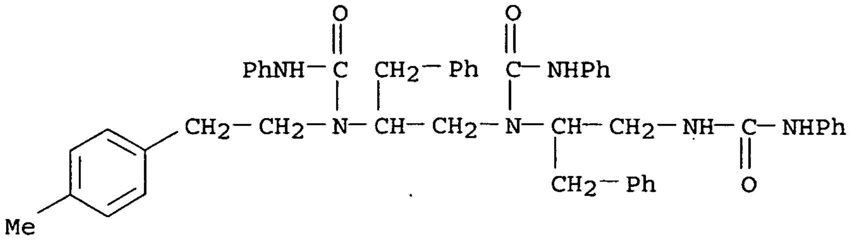
RN 537051-27-7 CAPLUS
CN Urea, N-[2-[ethyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 537051-28-8 CAPLUS
CN Urea, N-[2-[[2-[4-(2-methylpropyl)phenyl]propyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

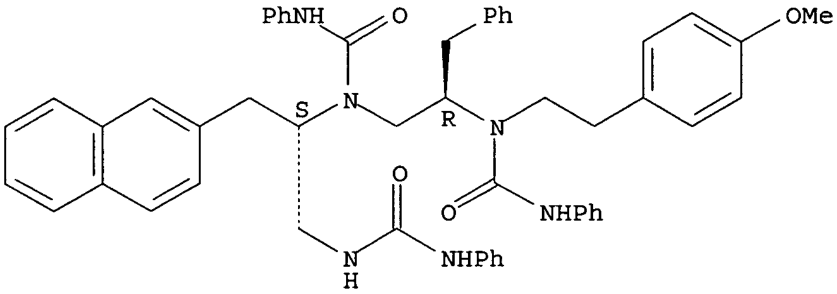


RN 537051-29-9 CAPLUS
CN Urea, N-[2-[[2-(4-methylphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)



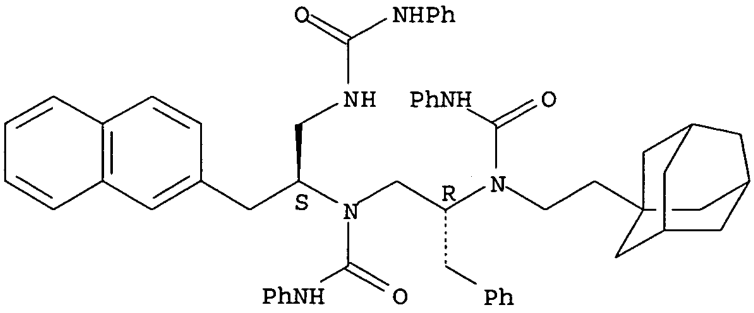
RN 537052-67-8 CAPLUS
CN Urea, N-[(2R)-2-[[2-(4-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N-[(1S)-1-(2-naphthalenylmethyl)-2-[[(phenylamino)carbonyl]amino]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



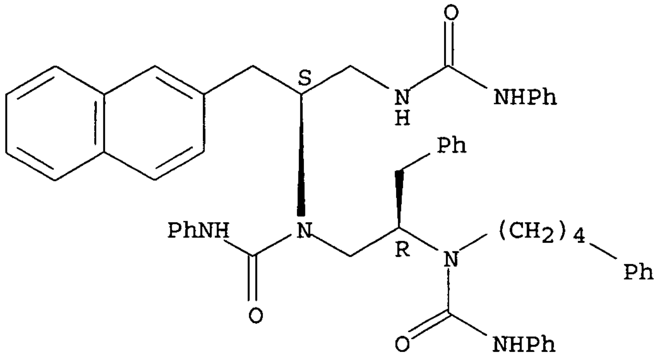
RN 537052-68-9 CAPLUS
CN Urea, N-[(1S)-1-(2-naphthalenylmethyl)-2-[[(phenylamino)carbonyl]amino]ethyl]-N'-phenyl-N-[(2R)-3-phenyl-2-[[(phenylamino)carbonyl](2-tricyclo[3.3.1.13,7]dec-1-ylethyl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537052-69-0 CAPLUS
CN Urea, N-[(1S)-1-(2-naphthalenylmethyl)-2-[[(phenylamino)carbonyl]amino]ethyl]-N'-phenyl-N-[(2R)-3-phenyl-2-[[(phenylamino)carbonyl](4-phenylbutyl)amino]propyl]- (9CI) (CA INDEX NAME)

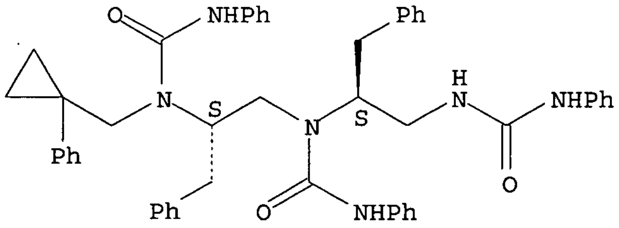
Absolute stereochemistry.



RN 537052-83-8 CAPLUS

CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl][(1-phenylcyclopropyl)methyl]amino]propyl]- (9CI) (CA INDEX NAME)

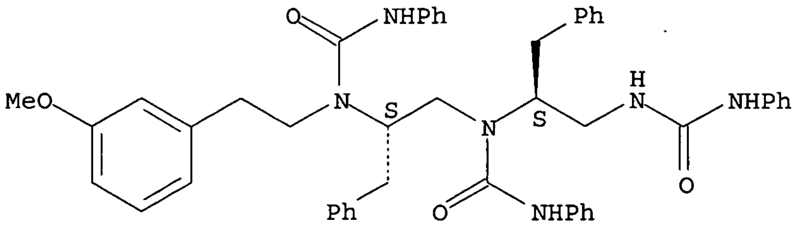
Absolute stereochemistry.



RN 537052-84-9 CAPLUS

CN Urea, N-[(2S)-2-[[2-(3-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

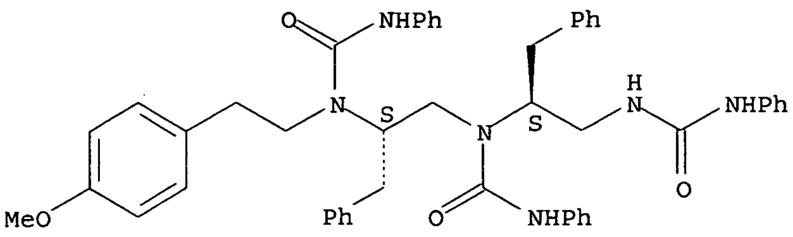
Absolute stereochemistry.



RN 537052-85-0 CAPLUS

CN Urea, N-[(2S)-2-[[2-(4-methoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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N
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MeO
Ph
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NHPh
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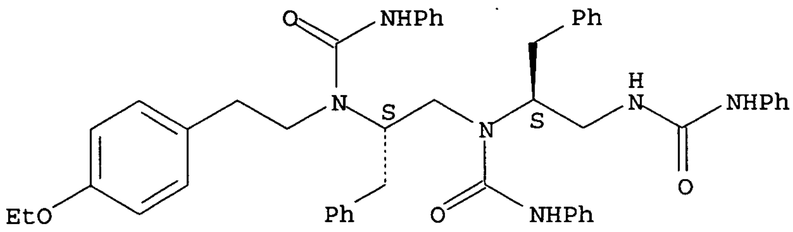
RN 537052-86-1 CAPLUS
CN Urea, N-[(2S)-2-[[2-(4-ethoxyphenyl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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EtO
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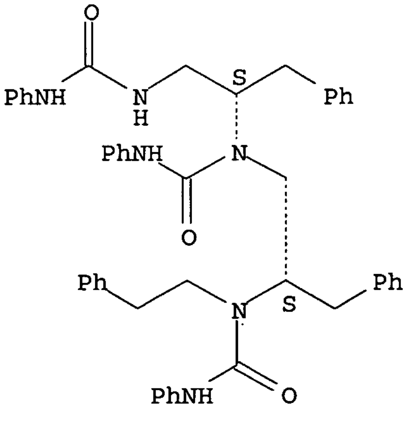
RN 537052-87-2 CAPLUS
CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl](2-phenylethyl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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S
Ph
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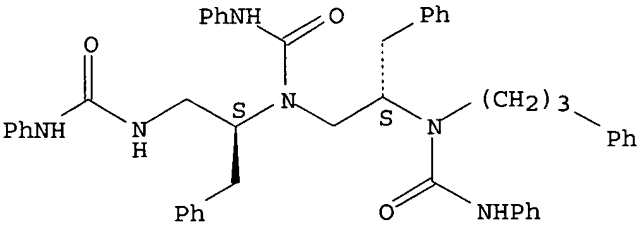
O

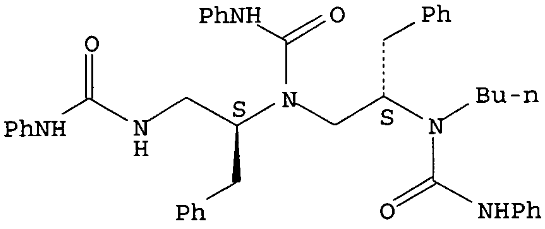
RN 537052-88-3 CAPLUS
CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl](3-phenylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



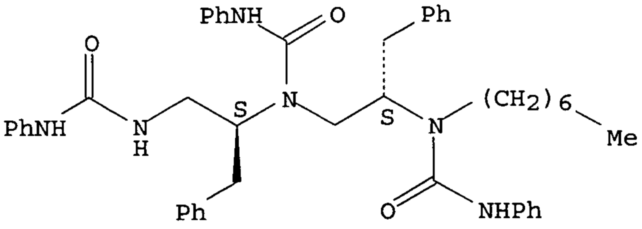
RN 537052-89-4 CAPLUS
CN Urea, N-[(2S)-2-[butyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



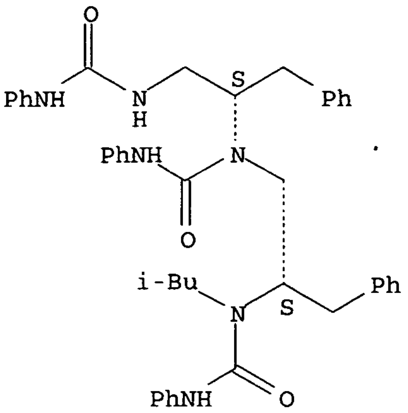
RN 537052-90-7 CAPLUS
CN Urea, N-[(2S)-2-[heptyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537052-91-8 CAPLUS
CN Urea, N-[(2S)-2-[(2-methylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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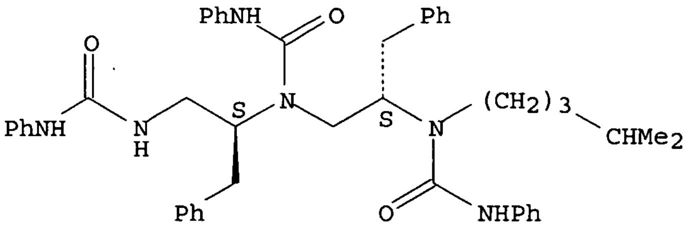
RN 537052-92-9 CAPLUS
CN Urea, N-[(2S)-2-[(4-methylpentyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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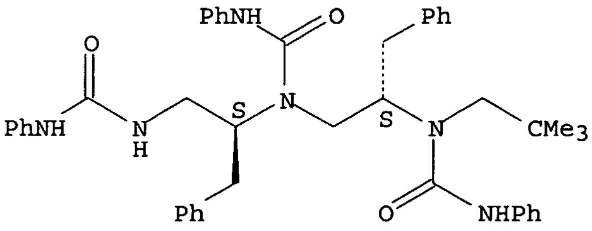
CN Urea, N-[(2S)-2-[(2,2-dimethylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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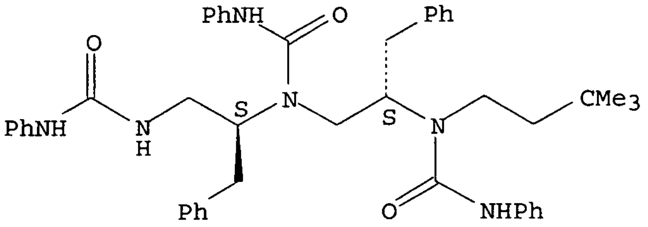
CN Urea, N-[(2S)-2-[(3,3-dimethylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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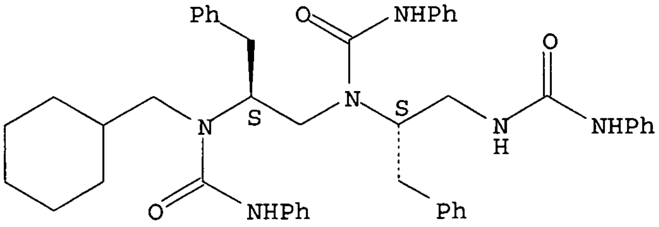
CN Urea, N-[(2S)-2-[(cyclohexylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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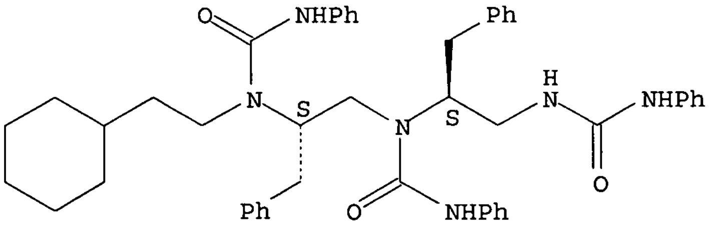
RN 537052-96-3 CAPLUS
CN Urea, N-[(2S)-2-[(2-cyclohexylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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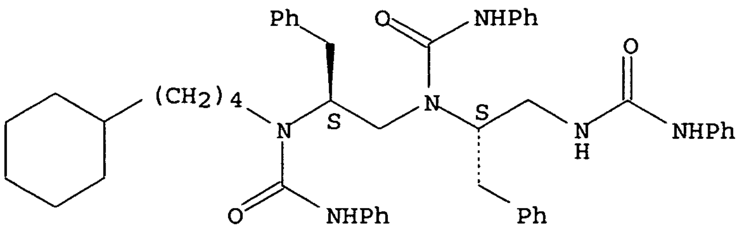
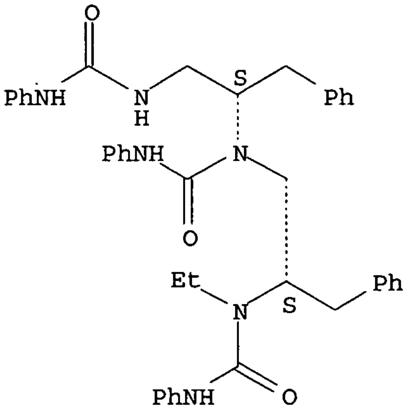
RN 537052-97-4 CAPLUS
CN Urea, N-[(2S)-2-[(4-cyclohexylbutyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



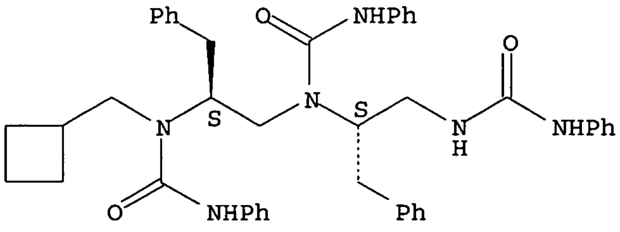
RN 537052-98-5 CAPLUS
CN Urea, N-[(2S)-2-[ethyl[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



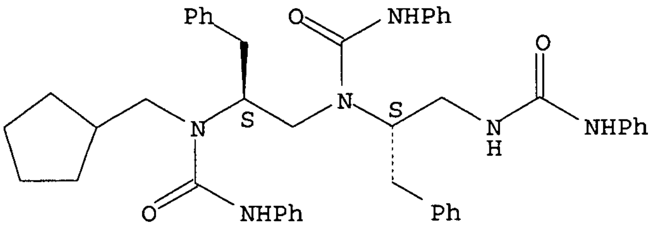
RN 537052-99-6 CAPLUS
CN Urea, N-[(2S)-2-[(cyclobutylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-00-2 CAPLUS
CN Urea, N-[(2S)-2-[(cyclopentylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

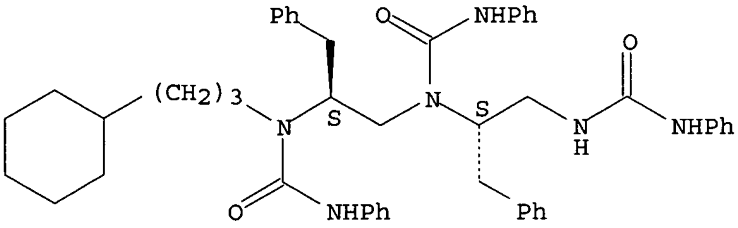
Absolute stereochemistry.



RN 537053-01-3 CAPLUS

CN Urea, N-[(2S)-2-[(3-cyclohexylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

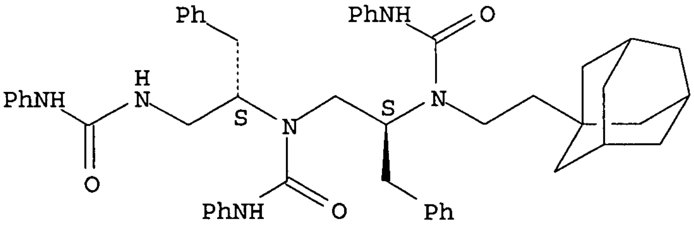
Absolute stereochemistry.



RN 537053-02-4 CAPLUS

CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl](2-tricyclo[3.3.1.13,7]dec-1-ylethyl)amino]propyl]- (9CI) (CA INDEX NAME)

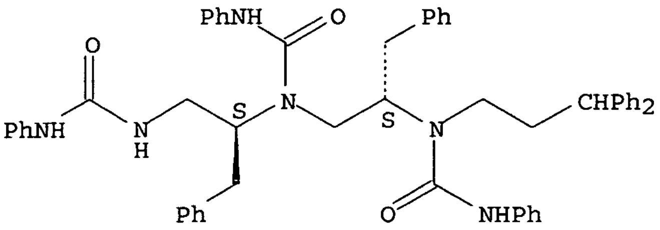
Absolute stereochemistry.



RN 537053-03-5 CAPLUS

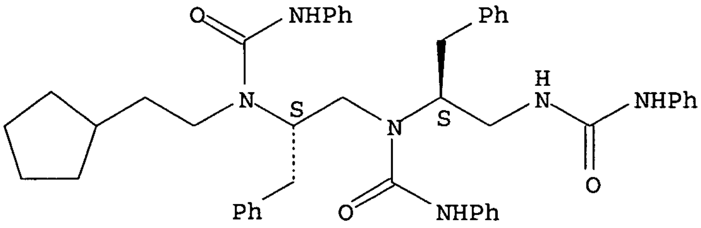
CN Urea, N-[(2S)-2-[(3,3-diphenylpropyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-04-6 CAPLUS
CN Urea, N-[(2S)-2-[(2-cyclopentylethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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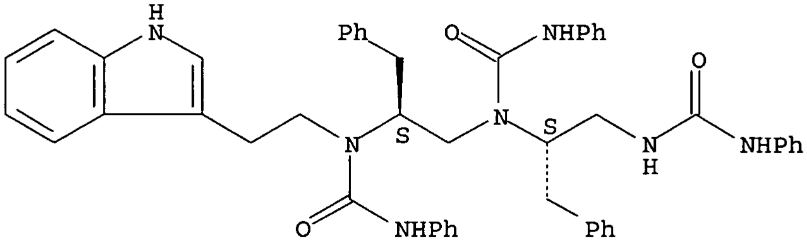
CN Urea, N-[(2S)-2-[[2-(1H-indol-3-yl)ethyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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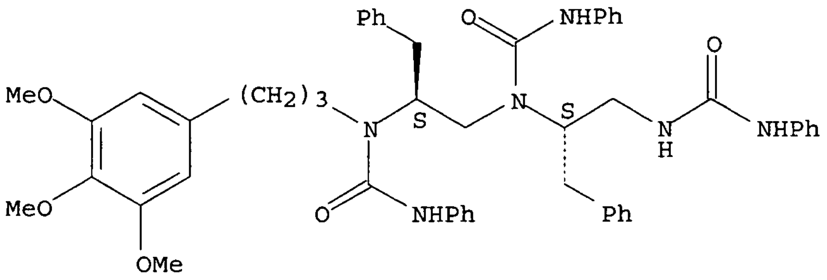
CN Urea, N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]-N-[(2S)-3-phenyl-2-[[(phenylamino)carbonyl][3-(3,4,5-trimethoxyphenyl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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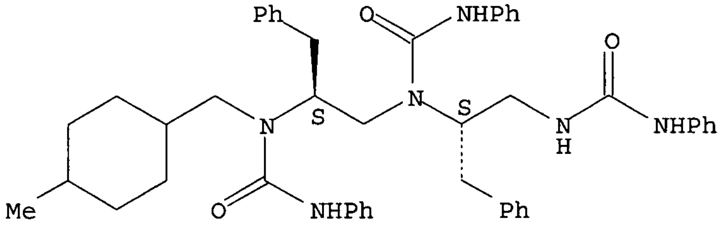
CN Urea, N-[(2S)-2-[[(4-methylcyclohexyl)methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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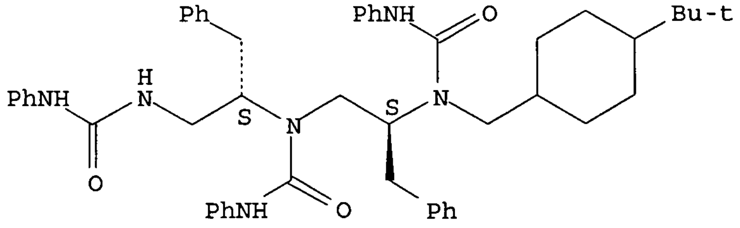
CN Urea, N-[(2S)-2-[[[4-(1,1-dimethylethyl)cyclohexyl]methyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 540529-37-1 CAPLUS
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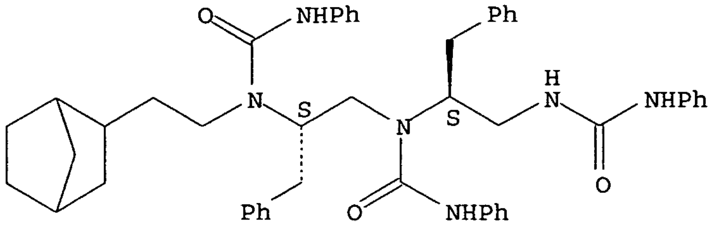
Absolute stereochemistry.



Not in Pat's

L12 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

2 APPs

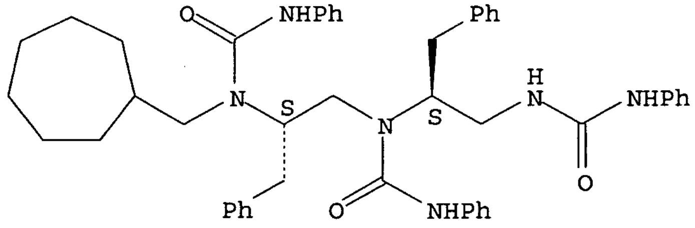
ACCESSION NUMBER: 2000:498548 CAPLUS
DOCUMENT NUMBER: 133:252127
TITLE: An efficient two-step synthesis of mono-, di- and triureas from resin-bound amides
AUTHOR(S): Nefzi, A.; Ong, N. A.; Houghten, R. A.
CORPORATE SOURCE: Torrey Pines Institute for Molecular Studies, San Diego, CA, 92121, USA
SOURCE: Tetrahedron Letters (2000), 41(29), 5441-5446
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:252127

AB An efficient method for the solid-phase synthesis of mono-, di-, and triureas from resin-bound mono-, di-, and triamines is described. The exhaustive reduction of solid support-bound amides generated the requisite amines, which, following treatment with isocyanates and cleavage, provided the corresponding ureas in high purity and good yields.

IT 295343-36-1P 295343-40-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of mono-, di- and triureas from resin-bound amides)

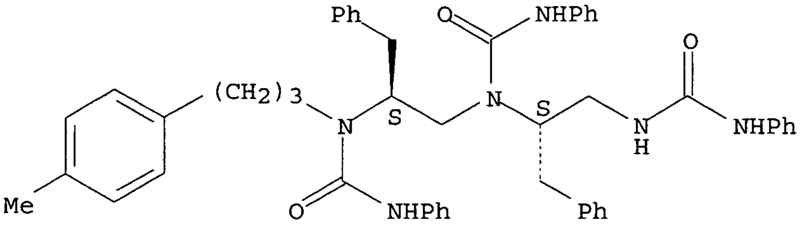
RN 295343-36-1 CAPLUS
CN Urea, N-[(2S)-2-[(cycloheptylmethyl)[(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 295343-40-7 CAPLUS
CN Urea, N-[(2S)-2-[[3-(4-methylphenyl)propyl][(phenylamino)carbonyl]amino]-3-phenylpropyl]-N'-phenyl-N-[(1S)-2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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REFERENCE COUNT:         25    THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> fil caol;s 17
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                                                          ENTRY    SESSION
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FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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  assignees, and patent information, e.g., patent numbers, are
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L13          0 L7

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L4               STR L1
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L6               STR L4
L7            65 SEARCH L6  SUB=L5 FUL
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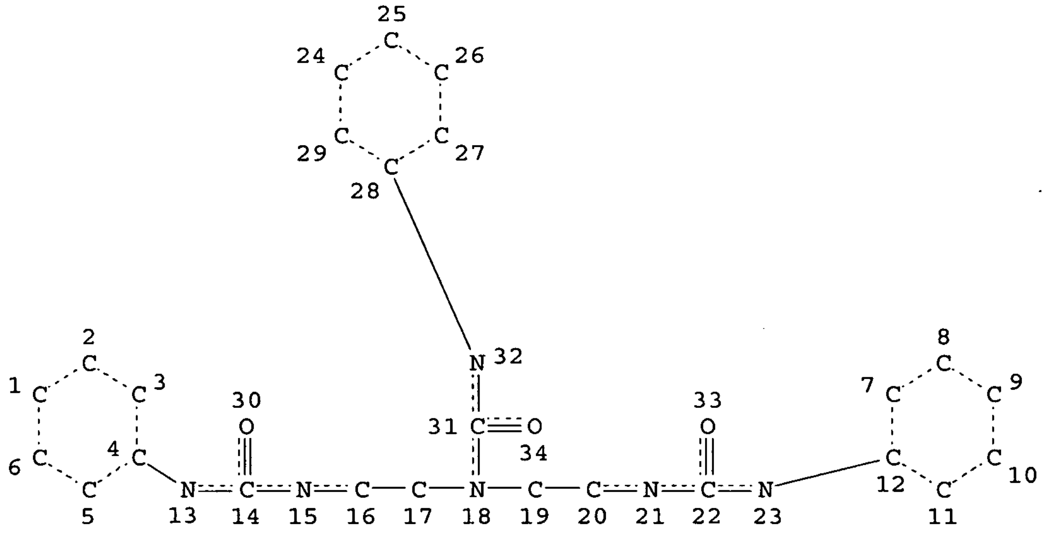

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O
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C
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C
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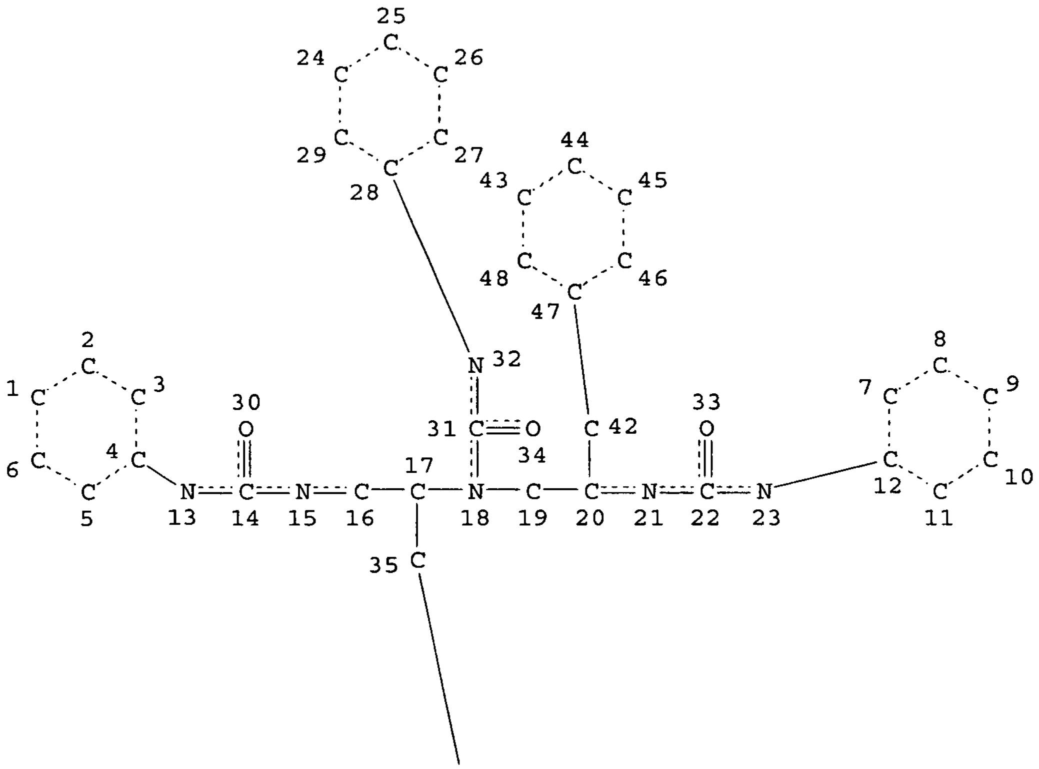
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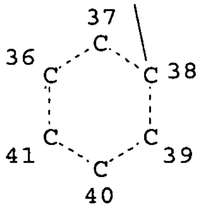
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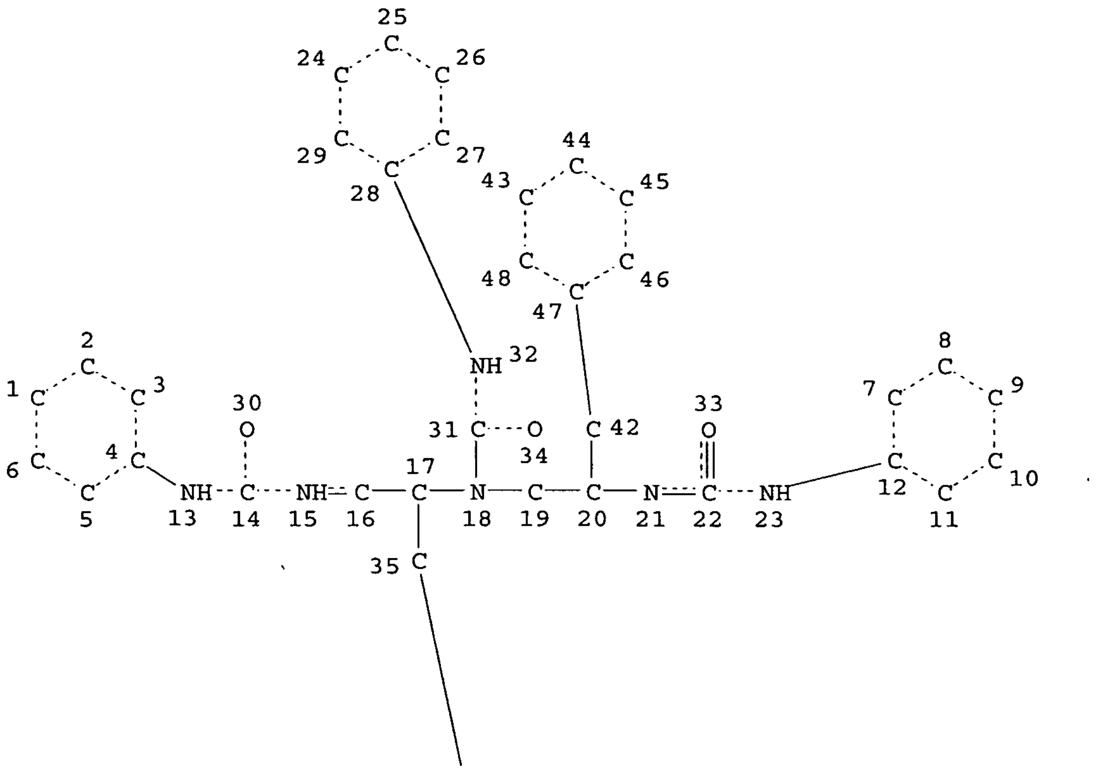
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

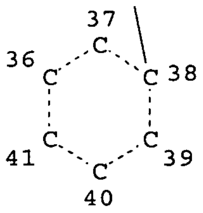
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

```
L5            65 SEA FILE=REGISTRY SUB=L3 SSS FUL L4
L6               STR
```


25
24 C C 26
29 C C 27
28
44
43 C C 45
48 C C 46
47
2
1 C C 3
6 C 4 C
5
8
7 C C 9
C 12 C 10
11
NH 32
30 O
31 C O 34
C 42
33 O
NH C NH C C N C C N C NH
13 14 15 16 17 18 19 20 21 22 23
35 C

Page 1-A


37
36 C C 38
41 C C 39
40

```
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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
L7             65 SEA FILE=REGISTRY SUB=L5 SSS FUL L6

100.0% PROCESSED      65 ITERATIONS                              65 ANSWERS
SEARCH TIME: 00.00.01


=> log y
COST IN U.S. DOLLARS                                      SINCE FILE       TOTAL
```

```
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.44     275.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE     TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00      -2.25

STN INTERNATIONAL LOGOFF AT 14:28:37 ON 08 AUG 2006
```